On the parabolic kernel of the Schrödinger operator

by

PETER LI([1])   and   SHING TUNG YAU

University of Utah   *University of California, San Diego*
Salt Lake City, UT, U.S.A.   *La Jolla, CA, U.S.A.*

Table of contents

§ 0. Introduction

In this paper, we will study parabolic equations of the type

$$\left(\Delta - q(x, t) - \frac{\partial}{\partial t}\right) u(x, t) = 0 \tag{0.1}$$

on a general Riemannian manifold. The function $q(x, t)$ is assumed to be C^2 in the first variable and C^1 in the second variable. In classical situations [20], a Harnack inequality for positive solutions was established locally. However, the geometric dependency of the estimates is complicated and sometimes unclear. Our goal is to prove a Harnack inequality for positive solutions of (0.1) (§ 2) by utilizing a gradient estimate derived in § 1. The method of proof is originated in [26] and [8], where they have studied the elliptic case, i.e. the solution is time independent. In some situations (Theorems 2.2 and

---

2.3), the Harnack inequality is valid globally, which enables us to relate the global geometry with the analysis.

In §3, we apply the Harnack inequality to obtain upper estimates for the fundamental solution of the equation

$$\left(\Delta - q(x) - \frac{\partial}{\partial t}\right) u(x, t) = 0, \tag{0.2}$$

where q is a function on M alone. We shall point out that for the heat equation ($q=0$), upper estimates for the heat kernel were obtained in [7] and [5]. However the estimate which we obtain is so far the sharpest, especially for large time. When the Ricci curvature is nonnegative the sharpness is apparent, since a comparable lower bound is also obtained in §4. A lower bound for the fundamental solution of (0.2) is also derived for some special situations.

Applications of these estimates for the heat kernel are discussed in §5. A generalization of Widder's [25] uniqueness theorem for positive solutions of the heat equation is proved([2]) (Theorem 5.1). In fact, the condition on the curvature is best possible due to the counter-example of Azencott [2]. We also point out that generalizations of Widder's theorem to general elliptic operators in $\mathbf{R}^n$ were derived in [21], [11] and [1].

When M has nonnegative Ricci curvature, sharp upper and lower bounds of Green's function are derived. This can also be viewed as a necessary and sufficient condition for the existence of Green's function which was studied in [23]. In fact, in [24], our estimates on Green's function were proved for nonnegatively Ricci curved manifolds with pole and with nonnegative radial sectional curvatures. In [13], Gromov proved lower bounds for all the eigenvalues of the Laplacian on a compact nonnegatively Ricci curved manifold without boundary. We generalized these estimates to allow the manifold to have convex boundaries with either Dirichlet or Neumann boundary conditions. These lower bounds can also be viewed as a generalization of the lower bound for the first eigenvalue obtained in [16].

Another application is to derive an upper bound of the first Betti number, b_1, on a compact manifold in terms of its dimension, a lower bound of the Ricci curvature, and an upper bound of the diameter. The manifold is allowed to have convex boundaries, in which case b_1 can be taken to be the dimension of either $H^1(M)$ of $H^1(M, \partial M)$. It was proved in [14] that if M has no boundary, then b_k can be estimated from above by the

---

([2]) During the preparation of this paper, H. Donnelly has independently found a different proof of the uniqueness theorem when the Ricci curvature of M is bounded from below.

dimension, k, a lower bound of the sectional curvature, and an upper bound of the diameter.[3] On b_k, for $k>1$, we derived a weaker estimate than that in [14] assuming both upper bound of the sectional curvature and lower bound of the Ricci curvature. However, in this case, the manifold is also allowed to have nonempty convex boundaries. Some of our estimates on the Betti numbers overlap with results in [17], [18], and [19].

Finally, in §6, we study the asymptotic behaviour for the fundamental solution of the operator $\Delta - \lambda^2 q(x) - \partial/\partial t$ as $\lambda \to \infty$. This formula was needed in [22] for the understanding of multiple-welled potentials. In fact, the results in [22] can be carried over to any complete manifold after applying the formula in Theorem 6.1.

§1. Gradient estimates

Throughout this section, M is assumed to be an n-dimensional complete Riemannian manifold with (possibly empty) boundary, ∂M. Let $\partial/\partial v$ be the outward pointing unit normal vector to ∂M, and denote the second fundamental form of ∂M with respect to $\partial/\partial v$ by II.

Our goal is to derive estimates on the derivates of positive solutions $u(x, t)$ on $M \times (0, \infty)$ of the equation

$$\left(\Delta - q(x, t) - \frac{\partial}{\partial t}\right) u(x, t) = 0. \tag{1.1}$$

In general, these estimates are of interior nature. However, in some cases, they can be extended to be global estimates which hold up to the boundary. First, we will prove the following lemma which is essential in the derivation of our gradient estimates.

LEMMA 1.1. *Let $f(x, t)$ be a smooth function defined on $M \times [0, \infty)$ satisfying*

$$\left(\Delta - \frac{\partial}{\partial t}\right) f = -|\nabla f|^2 + q, \tag{1.2}$$

where q is a C^2 function defined on $M \times (0, \infty)$. For any given $\alpha \geq 1$, the function

$$F = t(|\nabla f|^2 - \alpha f_t - \alpha q) \tag{1.3}$$

satisfies the inequality

$$\left(\Delta - \frac{\partial}{\partial t}\right) F \geq -2\langle \nabla f, \nabla F \rangle - \frac{1}{t} F - 2Kt|\nabla f|^2$$
$$+ \frac{2t}{n}(|\nabla f|^2 - f_t - q)^2 - \alpha t \Delta q - 2(\alpha - 1) t \langle \nabla f, \nabla g \rangle, \tag{1.4}$$

where $-K(x)$, with $K(x) \geq 0$, is a lower bound of the Ricci curvature tensor of M at the point $x \in M$, and the subscript t denotes partial differentiation with respect to the t-variable.

Proof. Let $e_1, e_2, \ldots, e_n$ be a local orthonormal frame field on M. We adopt the notation that subscripts in $i, j,$ and k, with $1 \leq i, j, k \leq n$, mean covariant differentiations in the e_i, e_j and e_k directions respectively.

Differentiating (1.3) in the direction of e_i, we have

$$F_i = t(2f_j f_{ji} - \alpha f_{ti} - \alpha q_i),$$

where the summation convention is adopted on repeated indices. Differentiating once more in the e_i direction and summing over $i = 1, 2, \ldots, n$, we obtain

$$\Delta F = t(2f_{ji}^2 + 2f_j f_{jii} - \alpha f_{tii} - \alpha q_{ii})$$
$$\geq t\left[\frac{2}{n}(\Delta f)^2 + 2\langle \nabla f, \nabla \Delta f \rangle - 2K|\nabla f|^2 - \alpha(\Delta f)_t - \alpha \Delta q\right],$$

where we have used the inequalities

$$\sum_{i,j} f_{ij}^2 \geq \frac{(f_{ii})^2}{n},$$

and

$$f_j f_{jii} = f_j f_{iij} + R_{ij} f_i f_j \geq \langle \nabla f, \nabla \Delta f \rangle - K|\nabla f|^2.$$

Applying the formula

$$\Delta f = -|\nabla f|^2 + q + f_t = -\frac{1}{t} F - (\alpha - 1)(q + f_t),$$

we conclude,

$$\Delta F \geq \frac{2t}{n}(|\nabla f|^2 - f_t - q)^2 - 2\langle \nabla f, \nabla F \rangle - 2(\alpha - 1) t \langle \nabla f, \nabla(f_t) \rangle$$

$$- 2(\alpha - 1) t \langle \nabla f, \nabla q \rangle - 2Kt|\nabla f|^2 + \alpha F_t - \alpha(|\nabla f|^2 - \alpha f_t - \alpha q)$$

$$+\alpha(\alpha-1)\,tf_{tt}+\alpha(\alpha-1)\,tq_t-\alpha t\Delta q$$

$$=\frac{2t}{n}(|\nabla f|^2-f_t-q)^2-2\langle\nabla f,\nabla F\rangle+F_t-(|\nabla f|^2-\alpha f_t-\alpha q)$$

$$-2Kt|\nabla f|^2-\alpha t\Delta q-2(\alpha-1)\,t\langle\nabla f,\nabla q\rangle.$$

This proves the lemma.

THEOREM 1.1. *Let M be a compact manifold with nonnegative Ricci curvature. Suppose the boundary of M is convex, i.e. II$\geqslant$0, whenever $\partial M\neq\varnothing$. Let u(x, t) be a nonnegative solution of the heat equation*

$$\left(\Delta-\frac{\partial}{\partial t}\right)u(x,\,t)=0$$

on M$\times$(0, ∞), with Neumann boundary condition

$$\frac{\partial u}{\partial v}=0$$

on $\partial M\times$(0, ∞). Then u satisfies the estimate

$$\frac{|\nabla u|^2}{u^2}-\frac{u_t}{u}\leqslant\frac{n}{2t}$$

on M$\times$(0, ∞).

Proof. By setting $f=\log(u+\varepsilon)$ for $\varepsilon>0$, one verifies that f satisfies

$$\left(\Delta-\frac{\partial}{\partial t}\right)f=-|\nabla f|^2.$$

Applying Lemma 1.1 to f by setting $\alpha=1$, $q=0$, and $K=0$, we have

$$\left(\Delta-\frac{\partial}{\partial t}\right)F\geqslant-2\langle\nabla f,\nabla F\rangle+\frac{2}{nt}F\left(F-\frac{n}{2}\right).\tag{1.5}$$

The theorem claims that F is at most $n/2$. If not, at the maximum point (x_0, t_0) of F on $M\times[0, T]$ for some $T>0$,

$$F(x_0,\,t_0)>\frac{n}{2}>0.$$

Clearly, $t_0>0$, because $F(x, 0)=0$. If x_0 is an interior point of M, then by the fact that (x_0, t_0) is a maximum point of F in $M\times[0, T]$, we have

$$\Delta F(x_0, t_0) \leqslant 0,$$

$$\nabla F(x_0, t_0) = 0,$$

and

$$F_t(x_0, t_0) \geqslant 0.$$

Combining with (1.5), this implies

$$0 \geqslant \frac{2}{nt_0} F(x_0, t_0) \left(F(x_0, t_0) - \frac{n}{2} \right),$$

which is a contradiction. Hence x_0 must be on ∂M.

In this case, since F satisfies (1.5), the strong maximum principle yields

$$\frac{\partial F}{\partial \nu}(x_0, t_0) > 0. \tag{1.6}$$

However

$$\frac{\partial F}{\partial \nu} = 2f_j f_{j\nu} - f_{t\nu} = 2 \sum_{\alpha=1}^{n-1} f_\alpha f_{\alpha\nu},$$

since $f_\nu = u_\nu/(u+\varepsilon) = 0$ on ∂M, and we are assuming that $e_n = \partial/\partial\nu$. Computing $f_{\alpha\nu}$ in terms of the second fundamental form $II = (h_{\alpha\beta})$, we conclude that

$$\frac{\partial F}{\partial \nu} = -2 \sum_{\alpha,\beta=1}^{n-1} h_{\alpha\beta} f_\alpha f_\beta = -2II(\nabla f, \nabla f).$$

Inequality (1.6) and the convexity assumption on ∂M yield a contradiction. Hence

$$F \leqslant \frac{n}{2},$$

and the theorem follows by letting $\varepsilon \to 0$.

THEOREM 1.2. *Let M be a complete manifold with boundary, ∂M. Assume $p \in M$ and let $B_p(2R)$ to be a geodesic ball of radius $2R$ around p which does not intersect ∂M. We denote $-K(2R)$, with $K(2R) \geqslant 0$, to be a lower bound of the Ricci curvature on $B_p(2R)$. Let $q(x, t)$ be a function defined on $M \times [0, T]$ which is C^2 in the x-variable and C^1 in the t-variable. Assume that*

$$\Delta q \leqslant \theta(2R)$$

and

$$|\nabla q| \leqslant \gamma(2R)$$

on $B_p(2R) \times [0, T]$ *for some constants* $\theta(2R)$ *and* $\gamma(2R)$. *If* $u(x, t)$ *is a positive solution of the equation*

$$\left(\Delta - q - \frac{\partial}{\partial t}\right) u(x, t) = 0$$

on $M \times (0, T]$, *then for any* $\alpha > 1$ *and* $\varepsilon \in (0, 1)$, $u(x, t)$ *satisfies the estimate*

$$\frac{|\nabla u|^2}{u^2} - \frac{\alpha u_t}{u} - \alpha q \leqslant C_3 \alpha^2 R^{-2}(1 + R\sqrt{K} + \alpha^2(\alpha-1)^{-1}) + \frac{n}{2}\alpha^2 t^{-1}$$

$$+ \left[C_4(\gamma^4(\alpha-1)^2\alpha^4\varepsilon^{-1})^{1/3} + \frac{n^2}{2}(1-\varepsilon)^{-1}\alpha^4(\alpha-1)^{-2}K^2 + \frac{n}{2}\alpha^3\theta \right]^{1/2}$$

on $B_p(R)$, *where* C_3 *and* C_4 *are constants depending only on* n.

Proof. As in the proof of Theorem 1.1, we define the function

$$F(x, t) = t(|\nabla f|^2 - \alpha f_t - \alpha q)$$

where

$$f = \log u.$$

Let $\bar\varphi(r)$ be a C^2 function defined on $[0, \infty)$ such that

$$\bar\varphi(r) = \begin{cases} 1 & \text{if } r \in [0, 1] \\ 0 & \text{if } r \in [2, \infty), \end{cases}$$

with

$$0 \geqslant \frac{\bar\varphi'(r)}{\bar\varphi^{1/2}(r)} \geqslant -C_1,$$

and

$$\bar\varphi''(r) \geqslant -C_2,$$

for some constants $C_1, C_2 > 0$. If $r(x)$ denotes the distance beween p and x, we set

$$\varphi(x) = \bar\varphi\left(\frac{r(x)}{R}\right).$$

We consider the function φF, with support in $B_p(2R) \times [0, \infty)$, which is in general, only Lipschitz since $r(x)$ is only Lipschitz on the cut locus of p. However, an argument of Calabi, which was also used in [8], allows us to assume without loss of generality that φF is smooth when applying the maximum principle.

Let (x_0, t_0) be a point in $M \times [0, T]$ at which φF achieves its maximum. Clearly, we may assume φF is positive at (x_0, t_0), or else the theorem follows trivially. At (x_0, t_0), we have

$$\nabla(\varphi F) = 0,$$

$$\frac{\partial(\varphi F)}{\partial t} \geq 0,$$

and

$$\Delta(\varphi F) \leq 0.$$

By a comparison theorem in Riemannian geometry,

$$\Delta \varphi = \frac{\bar{\varphi}' \Delta r}{R} + \frac{\bar{\varphi}'' |\nabla r|^2}{R^2}$$

$$\geq -\frac{C_1}{R}(n-1)\sqrt{K} \coth(R\sqrt{K}) - \frac{C_2}{R^2}.$$

Applying Lemma 1 to the equation

$$\Delta(\varphi F) = (\Delta \varphi) F + 2\langle \nabla \varphi, \nabla F \rangle + \varphi(\Delta F),$$

and using the above inequality, we arrive at

$$\Delta(\varphi F) \geq -F(C_1 R^{-1}(n-1)\sqrt{K} \coth(R\sqrt{K}) + C_2 R^{-2})$$

$$+ 2\langle \nabla \varphi, \nabla(\varphi F) \rangle \varphi^{-1} + \varphi \left[F_t - 2\langle \nabla f, \nabla F \rangle \right.$$

$$+ \frac{2}{n} t(|\nabla f|^2 - f_t - q)^2 - t^{-1}F - 2Kt|\nabla f|^2$$

$$\left. - \alpha t \Delta q - 2(\alpha-1)t\langle \nabla f, \nabla q \rangle \right] - 2F|\nabla \varphi|^2 \varphi^{-1}.$$

Evaluating at (x_0, t_0) yields

$$0 \geq -F(C_1 R^{-1}(n-1)\sqrt{K} \coth(R\sqrt{K}) + C_2 R^{-2})$$

$$- 2F|\nabla \varphi|^2 \varphi^{-1} + 2F\langle \nabla f, \nabla \varphi \rangle + \frac{2}{n} t_0 \varphi(|\nabla f|^2 - f_t - q)^2 - \varphi t^{-1}F$$

$$- 2Kt_0 \varphi|\nabla f|^2 - \alpha \varphi t_0 \Delta q - 2(\alpha-1)t_0 \varphi\langle \nabla f, \nabla q \rangle.$$

Multiplying through by φt_0 and using the assumptions on Δq and $|\nabla q|$ with the estimate on $|\nabla \varphi|$, this becomes

$$0 \geqslant t_0 \varphi F \left[-C_1 R^{-1}(n-1)\sqrt{K} \coth(R\sqrt{K}) - C_2 R^{-2} - 2C_1^2 R^{-2} - t_0^{-1} \right]$$

$$-2t_0 \varphi F |\nabla f| C_1 R^{-1} \varphi^{1/2} + \frac{2}{n} t_0^2 \varphi^2 \left[(|\nabla f|^2 - f_t - q)^2 - nK|\nabla f|^2 \right] \tag{1.7}$$

$$-\alpha t_0^2 \theta - 2(\alpha - 1) t_0^2 \gamma \varphi^{1/2} |\nabla f|.$$

If we let

$$y = \varphi |\nabla f|^2$$

and

$$z = \varphi(f_t + q),$$

and observe that

$$C_1 R^{-1}(n-1)\sqrt{K} \coth(R\sqrt{K}) + C_2 R^{-2} + 2C_1^2 R^{-2} \leqslant C_3 R^{-2}(1 + R\sqrt{K}),$$

for some constant C_3 depending only on n, (1.7) takes the form

$$0 \geqslant \varphi F \left[-t_0 C_3 R^{-2}(1 + R\sqrt{K}) - 1 \right] + \frac{2}{n} t_0^2$$

$$\times \left[(y-z)^2 - nC_1 R^{-1} y^{1/2}(y - \alpha z) - nKy - n(\alpha-1)\gamma y^{1/2} \right] - t_0^2 \alpha \theta. \tag{1.8}$$

On the other hand, we observe that

$$(y-z)^2 - nC_1 R^{-1} y^{1/2}(y - \alpha z) - nKy - n(\alpha-1)\gamma y^{1/2}$$

$$= (1-\varepsilon-\delta) y^2 - (2-\varepsilon\alpha) yz + z^2 + (\varepsilon y - nC_1 R^{-1} y^{1/2})(y - \alpha z) + \delta y^2 + nKy - n(\alpha-1)\gamma y^{1/2}$$

$$= \left(\alpha^{-1} - \frac{\varepsilon}{2} \right)(y - \alpha z)^2 + \left(1 - \varepsilon - \delta - \alpha^{-1} + \frac{\varepsilon}{2} \right) y^2 + \left(1 - \alpha + \frac{\varepsilon}{2} \alpha^2 \right) z^2 \tag{1.9}$$

$$+ (\varepsilon y - nC_1 R^{-1} y^{1/2})(y - \alpha z) + \delta y^2 - nKy - n(\alpha-1)\gamma y^{1/2}.$$

Setting $\delta = (\alpha^{-1} - 1)^2$ and $\varepsilon = 2 - 2\alpha^{-1} - 2(\alpha^{-1} - 1)^2$, we check that

$$1 - \varepsilon - \delta - \alpha^{-1} + \frac{\varepsilon}{2} = 0$$

and

$$1 - \alpha + \frac{\varepsilon}{2} \alpha^2 = 0.$$

Hence, (1.9) becomes

$$(y-z)^2 - nC_1 R^{-1} y^{1/2}(y - \alpha z) - nKy - n(\alpha-1)\gamma y^{1/2}$$

$$\geqslant \alpha^{-2}(y - \alpha z)^2 - C_3 \alpha^2 (\alpha-1)^{-1} R^{-2}(y - \alpha z) + \alpha^{-2}(\alpha-1)^2 y^2 - nKy - n(\alpha-1)\gamma y^{1/2}, \tag{1.10}$$

where we have used the fact that

$$2\alpha^{-2}(\alpha-1)y-nC_1R^{-1}y^{1/2}\geqslant -\frac{n^2}{8}C_1^2\alpha^2(\alpha-1)^{-1}R^{-2}$$

$$\geqslant -C_3\alpha^2(\alpha-1)^{-1}R^{-2}.$$

We will estimate the last three terms of (1.10) as follows,

$$\alpha^{-2}(\alpha-1)^2y^2-nKy-n(\alpha-1)\gamma y^{1/2}$$

$$\geqslant \alpha^{-2}(\alpha-1)^2y^2-(1-\varepsilon)\alpha^{-2}(\alpha-1)^2y^2-\frac{n^2}{2}(1-\varepsilon)^{-1}\alpha^2(\alpha-1)^{-2}K^2-n(\alpha-1)\gamma y^{1/2}$$

$$\geqslant \varepsilon\alpha^{-2}(\alpha-1)^2y^2-n(\alpha-1)\gamma y^{1/2}-\frac{n^2}{2}(1-\varepsilon)^{-1}\alpha^2(\alpha-1)^{-2}K^2$$

$$\geqslant -C_4(\gamma^4(\alpha-1)^2\alpha^2\varepsilon^{-1})^{1/3}-\frac{n^2}{2}(1-\varepsilon)^{-1}\alpha^2(\alpha-1)^{-2}K^2$$

for any $\varepsilon\in(0,1)$.

Combining this with (1.8) and (1.10), we conclude that

$$0\geqslant \varphi F[-t_0C_3R^{-2}(1+R\sqrt{K})-1]$$

$$+\frac{2}{n}[\alpha^{-2}(\varphi F)^2-C_3\alpha^2(\alpha-1)^{-1}R^{-2}\varphi Ft_0]$$

$$-\frac{2}{n}t_0^2\left[C_4(\gamma^4(\alpha-1)^2\alpha^2\varepsilon^{-1})^{1/3}+\frac{n^2}{2}(1-\varepsilon)^{-1}\alpha^2(\alpha-1)^{-2}K^2\right]-t_0^2\alpha\theta$$

$$=\frac{2}{n}\alpha^{-2}(\varphi F)^2-[C_3t_0R^{-2}(1+R\sqrt{K})+\alpha^2(\alpha-1)^{-1})+1](\varphi F)$$

$$-t_0^2\left[C_4(\gamma^4(\alpha-1)^2\alpha^2\varepsilon^{-1})^{1/3}+\frac{n^2}{2}(1-\varepsilon)^{-1}\alpha^2(\alpha-1)^{-2}K^2+\alpha\theta\right].$$

This implies that at the maximum point $(x_0, t_0)\in M\times[0, T]$,

$$\varphi F\leqslant C_3\alpha^2t_0R^{-2}(1+R\sqrt{K}+\alpha^2(\alpha-1)^{-1})+\frac{n}{2}\alpha^2$$

$$+t_0\left[C_4(\gamma^4(\alpha-1)^2\alpha^4\varepsilon^{-1})^{1/3}+\frac{n^2}{2}(1-\varepsilon)^{-1}\alpha^4(\alpha-1)^{-2}K^2+\frac{n}{2}\alpha^3\theta\right]^{1/2}.$$

In particular, on $M\times\{T\}$, F satisfies the estimate as claimed in the theorem for $\alpha>1$ and $0<\varepsilon<1$, since $t_0\leqslant T$.

THEOREM 1.3. *Let M be a complete manifold without boundary. Suppose u(x, t) is a positive solution on M×(0, T] of the equation*

$$\left(\Delta - q - \frac{\partial}{\partial t}\right) u(x, t) = 0.$$

Assume the Ricci curvature of M is bounded from below by $-K$, for some constant $K \geqslant 0$. We also assume that there exists a point $p \in M$, a constant θ, and a function $\gamma(r, t)$ such that

$$|\nabla q|(x, t) \leqslant \gamma(r(x), t)$$

and

$$\Delta q \leqslant \theta$$

on $M \times (0, T]$, where $r(x)$ denotes the distance from p to x. Then the following estimates hold:

(i) If $K = 0$ and

$$\lim_{r \to \infty} \frac{\gamma(r, t)}{r} \leqslant \tau(t),$$

then

$$\frac{|\nabla u|^2}{u^2} - \frac{u_t}{u} \leqslant \frac{n}{2} t^{-1} + q + C_5 \tau^{2/3}(t) + \left(\frac{n}{2} \theta\right)^{1/2}$$

on $M \times (0, T]$.

(ii) If $\gamma(r, t) \leqslant \gamma_0(t)$ for some function $\gamma_0(t)$, then

$$\frac{|\nabla u|^2}{u^2} - \frac{\alpha u_t}{u} \leqslant \alpha q + \frac{n}{2} \alpha^2 t^{-1} + C_6 [\gamma_0^{2/3}(t) + (\alpha - 1)^{-1} K + \theta^{1/2}]$$

on $M \times (0, T]$ for all $\alpha \in (1, 2)$.

Proof. To prove (i), we simply set $\alpha - 1 = R^{-2} \tau^{-1/2}(t)$ in Theorem 1.2, and let $R \to \infty$. As of (ii), we just let $R \to \infty$ without any substitution.

THEOREM 1.4. Let M be a compact manifold with Ricci curvature bounded from below by $-K$, for some constant $K \geqslant 0$. We assume that the boundary of M is convex, i.e. $II \geqslant 0$. If $u(x, t)$ is a positive solution on $M \times (0, \infty)$ of the heat equation

$$\left(\Delta - \frac{\partial}{\partial t}\right) u(x, t) = 0,$$

with Neumann boundary condition

$$\frac{\partial u}{\partial v} = 0$$

on $\partial M \times [0, \infty)$, *then* $u(x, t)$ *satisfies*

$$\frac{|\nabla u|^2}{u^2} - \frac{\alpha u_t}{u} \leq \frac{n}{\sqrt{2}} \alpha^2 (\alpha - 1)^{-1} K + \frac{n}{2} \alpha^2 t^{-1}$$

on $M \times (0, \infty)$, *for all* $\alpha > 1$.

Proof. This follows by combining the arguments in the proofs of Theorem 1.1 and Theorem 1.3.

COROLLARY 1.1. *Let M be a complete manifold without boundary. Suppose the Ricci curvature of M is nonnegative, and suppose q is a* C^2 *function defined on M with*

$$\Delta q \leq 0$$

and

$$|\nabla q| = o(r(x)),$$

where $r(x)$ *is the distance from x to some fixed point* $p \in M$. *If* $\inf q < 0$, *then the equation*

$$(\Delta - q) u(x) = 0$$

does not admit a positive solution on M. In particular,

$$\inf q = \inf \{ \operatorname{Spec} (\Delta - q) \},$$

where $\operatorname{Spec} (\Delta - q)$ *denotes the spectrum of the operator* $\Delta - q$.

Proof. Let $u(x)$ be a positive solution of $(\Delta - q) u = 0$. Applying Theorem 1.3 (i) to this time independent solution, we arrive at the estimate

$$\frac{|\nabla u|^2}{u^2} \leq \frac{n}{2t} + q.$$

Letting $t \to \infty$, and evaluating at a point where $q < 0$, we have a contradiction, unless $\inf q \geq 0$.

To prove the second half of the corollary, one observes that the quadratic form associated to $\Delta - q$ is given by

$$\frac{\int |\nabla u|^2 + \int q u^2}{\int u^2}$$

which is clearly bounded from below by $\inf q$. Hence

$$\inf\{\operatorname{Spec}(\Delta-q)\} \geqslant \inf q.$$

On the other hand, we know that for $\varepsilon > 0$, the equation

$$[\Delta-(q-\inf q-\varepsilon)]\,u = 0$$

has no positive solution, which implies

$$\inf\{\operatorname{Spec}(\Delta-q)\} \leqslant \inf q+\varepsilon$$

(see [10]). However, ε is arbitrary, which yields the desired equality.

COROLLARY 1.2. *Let M be a complete manifold without boundary. Suppose the Ricci curvature of M is bounded from below by $-K$, for some constant $K \geqslant 0$. Assume that q is a C^2 function on M with*

$$\Delta q \leqslant \theta$$

and

$$|\nabla q|\,(x) \leqslant \gamma(r(p,x)),$$

for some constant θ, and some function γ depending only on the distance, $r(p,x)$, to some fixed point $p \in M$. Then

$$\inf q \leqslant \inf\{\operatorname{Spec}(\Delta-q)\}$$

and

$$\inf\{\operatorname{Spec}(\Delta-q)\} \leqslant Q,$$

where Q is finite and is defined in the following cases:

(i) *If $K=0$, and $\lim_{r\to\infty} r^{-1}\gamma(r) \leqslant \tau$ for some constant τ, then*

$$Q = \inf q + C_5\,\tau^{2/3} + \left(\frac{n}{2}\theta\right)^{1/2}.$$

(ii) *If $\gamma(r) \leqslant \gamma_0$ for some constant γ_0, then*

$$Q = \alpha\inf q + C_6[\gamma_0^{2/3} + (\alpha-1)^{-1}K + \theta^{1/2}]$$

for $\alpha \in (1,2)$.

Proof. Following the proof of Corollary 1.1, we apply Theorem 1.3 to any positive solution φ of the equation

$$(\Delta - q)\varphi = -\lambda\varphi$$

for $\lambda > Q$.

§2. Harnack inequalities

We will utilize the gradient estimate in §1 to obtain Harnack inequalities for positive solutions of (1.1).

THEOREM 2.1. *Let M be a complete manifold with boundary, ∂M. Assume $p \in M$ and let $B_p(2R)$ be a geodesic ball of radius $2R$ centered at p which does not intersect ∂M. We denote $-K(2R)$, with $K(2R) \geqslant 0$, to be a lower bound of the Ricci curvature on $B_p(2R)$. Let $q(x, t)$ be a function defined on $M \times [0, T]$ which is C^2 in the x-variable and C^1 in the t-variable. Assume that*

$$\Delta q \leqslant \theta(2R)$$

and

$$|\nabla q| \leqslant \gamma(2R)$$

on $B_p(2R) \times [0, T]$ for some constants $\theta(2R)$ and $\gamma(2R)$. If $u(x, t)$ is a positive solution of the equation

$$\left(\Delta - q - \frac{\partial}{\partial t}\right)u(x, t) = 0$$

on $M \times (0, T]$, then for any $\alpha > 1$, $0 < t_1 < t_2 \leqslant T$, and $x, y \in B_p(R)$, we have the inequality

$$u(x, t_1) \leqslant u(y, t_2)\left(\frac{t_2}{t_1}\right)^{n\alpha/2} \exp(A(t_2 - t_1) + \varrho_{\alpha, R}(x, y, t_2 - t_1)),$$

where

$$A = C_7[\alpha R^{-1}\sqrt{K} + \alpha^3(\alpha - 1)^{-1}R^{-2} + \gamma^{2/3}(\alpha - 1)^{1/3}\alpha^{-1/3} + (\alpha\theta)^{1/2} + \alpha(\alpha - 1)^{-1}K]$$

and

$$\varrho_{\alpha, R}(x, y, t_2 - t_1) = \inf_{\gamma \in \Gamma(R)}\left\{\frac{\alpha}{4(t_2 - t_1)}\int_0^1 |\dot{\gamma}|^2\, ds + (t_2 - t_1)\int_0^1 q(\gamma(s), (1-s)t_2 + st_1)\, ds\right\},$$

with inf taken over all paths in $B_p(R)$ parametrized by $[0, 1]$ joining y to x.

Proof. Let γ be any curve given by $\gamma\colon[0,1]\to B_p(R)$, with $\gamma(0)=y$ and $\gamma(1)=x$. We define $\eta\colon[0,1]\to B_p(R)\times[t_1,t_2]$ by

$$\eta(s) = (\gamma(s), (1-s)\,t_2+st_1).$$

Clearly $\eta(0)=(y, t_2)$ and $\eta(1)=(x, t_1)$. Integrating $(d/ds)(\log u)$ along η, we get

$$\log u(x, t_1)-\log u(y, t_2)= \int_0^1 \left(\frac{d}{ds}\log u\right) ds$$

$$= \int_0^1 \{\langle\dot\gamma, \nabla(\log u)\rangle -(t_2-t_1)(\log u)_t\} \, ds.$$

Applying Theorem 1.2 to $-(\log u)_t$, this yields

$$\log\left(\frac{u(x, t_1)}{u(y, t_2)}\right) \leqslant \int_0^1 \left\{|\dot\gamma|\,|\nabla\log u|+(t_2-t_1)\left[A+\frac{n}{2}\,at^{-1}+q\right]-(t_2-t_1)\,a^{-1}|\nabla\log u|^2\,ds\right\}.$$

$$(2.1)$$

Viewing $|\nabla\log u|$ as a variable and the integrand as a quadratic in $|\nabla\log u|$, we observe that it can be dominated from above by

$$\frac{a|\dot\gamma|^2}{4(t_2-t_1)}+(t_2-t_1)\left[A+\frac{n}{2}\,at^{-1}+q\right].$$

Since $t=(1-s)\,t_2+st_1$, (2.1) gives

$$\log\left(\frac{u(x, t_1)}{u(y, t_2)}\right) \leqslant \int_0^1 \left\{\frac{a|\dot\gamma|}{4(t_2-t_1)}+(t_2-t_1)\,q(\gamma(s), (1-s)\,t_2+st_1)\right\} ds+\frac{na}{2}\log\left(\frac{t_2}{t_1}\right)+A(t_2-t_1).$$

The theorem follows by taking exponentials of the above inequality.

Obviously, applying Theorems 1.3 and 1.4 instead, the above method yields:

THEOREM 2.2. *Let M be a complete manifold without boundary. Suppose u(x, t) is a positive solution on $M\times(0, T]$ of the equation*

$$\left(\Delta-q-\frac{\partial}{\partial t}\right) u(x, t) = 0.$$

Assume the Ricci curvature of M is bounded from below by $-K$, for some constant $K\geqslant0$. We also assume that there exists a point $p\in M$, a constant θ, and a function $\gamma(r, t)$, such that

$$|\nabla q|(x, t) \leq \gamma(r(x), t)$$

and

$$\Delta q \leq \theta$$

on $M \times (0, T]$, where $r(x)$ denotes the distance from p to x. Then for any points $x, y \in M$, and $0 < t_1 < t_2 \leq T$, the following estimates are valid:

(i) *If $K = 0$ and*

$$\lim_{r \to \infty} \frac{\gamma(r, t)}{r} \leq \tau$$

for all $t \in [0, T]$, then

$$u(x, t_1) \leq u(y, t_2) \left(\frac{t_2}{t_1}\right)^{n/2} \exp\left(C_5(\tau^{2/3} + \theta^{1/2})(t_2 - t_1) + \varrho(x, y, t_2 - t_1)\right),$$

where

$$\varrho(x, y, t_2 - t_1) = \inf_{\gamma \in \Gamma} \left\{ \frac{1}{4(t_2 - t_1)} \int_0^1 |\dot\gamma|^2 \, ds + (t_2 - t_1) \int_0^1 q(\gamma(s), (1-s)t_2 + st_1) \, ds \right\},$$

with inf taken over all paths in M parametrized by $[0, 1]$ joining y to x.

(ii) *If $\gamma(r, t) \leq \gamma_0$ for some constant γ_0 in $M \times [0, T]$, then*

$$u(x, t_1) \leq u(y, t_2) \left(\frac{t_2}{t_1}\right)^{n\alpha/2} \exp\left(C_6(t_2 - t_1)(\gamma_0^{2/3} + \theta^{1/2} + (\alpha - 1)^{-1}K) + \varrho_\alpha(x, y, t_2 - t_1)\right)$$

for all $\alpha \in (1, 2)$, where

$$\varrho_\alpha(x, y, t_2 - t_1) = \inf_{\gamma \in \Gamma} \left\{ \frac{\alpha}{4(t_2 - t_1)} \int_0^1 |\dot\gamma|^2 \, ds + (t_2 - t_1) \int_0^1 q(\gamma(s), (1-s)t_2 + st_1) \, ds \right\}.$$

THEOREM 2.3. *Let M be a compact manifold with Ricci curvature bounded from below by $-K$, for some constant $K \geq 0$. We assume that the boundary of M is convex, i.e. $\mathrm{II} \geq 0$. Let $u(x, t)$ be a positive solution on $M \times (0, \infty)$ of the heat equation*

$$\left(\Delta - \frac{\partial}{\partial t}\right) u(x, t) = 0,$$

with Neumann boundary condition

$$\frac{\partial u}{\partial \nu} = 0$$

on $\partial M \times [0, \infty)$. Then for any $\alpha > 1$, x, $y \in M$, and $0 < t_1 < t_2$, we have

$$u(x, t_1) \leq u(y, t_2) \left(\frac{t_2}{t_1}\right)^{n\alpha/2} \exp\left(\frac{n\alpha}{\sqrt{2}}(\alpha-1)^{-1}K(t_2-t_1)+\frac{\alpha r^2(x, y)}{4(t_2-t_1)}\right),$$

where $r(x, y)$ is the distance between x and y.

A mean value type inequality can be easily derived by averaging the function over any set in either the x-variable or the y-variable. In fact, this will be the form which we utilize most in the latter sections. For example, a corresponding mean value inequality of Theorem 2.3 will read

$$u(x, t_1) \leq \left(\fint_{B_x(R)} u^p(y, t_2)\right)^{1/p} \left(\frac{t_2}{t_1}\right)^{n\alpha/2} \exp\left(\frac{n\alpha}{\sqrt{2}}(\alpha-1)^{-1}K(t_2-t_1)+\frac{\alpha R^2}{4(t_2-t_1)}\right).$$

We also remark that from the definitions of ϱ's, they clearly satisfy the following relations:

$$\varrho_{\alpha, \infty}(x, y, t_2-t_1) = \varrho_\alpha(x, y, t_2-t_1), \tag{2.2}$$

$$\varrho_{1, \infty}(x, y, t_2-t_1) = \varrho_1(x, y, t_2-t_1) = \varrho(x, y, t_2-t_1), \tag{2.3}$$

and

$$\varrho_\alpha(x, y, t_2-t_1) = \frac{\alpha r^2(x, y)}{4(t_2-t_1)} \tag{2.4}$$

if $q \equiv 0$.

COROLLARY 2.1. *Let M be a compact manifold with non-negative Ricci curvature. If $\partial M \neq \emptyset$, we assume that it must be convex. The Neumann heat kernel on M must satisfy*

$$H(x, y, t) \geq (4\pi t)^{-n/2} \exp\left(\frac{-r^2(x, y)}{4t}\right).$$

In particular, the Neumann eigenvalues μ_i of M satisfy

$$\sum_{i=0}^{\infty} e^{-\mu_i t} \geq (4\pi t)^{-n/2}V(M).$$

Proof. Apply Theorem 2.3 to the function

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

gives

$$H(x, x, t_1) \leqslant H(x, y, t_2) \left(\frac{t_2}{t_1}\right)^{n/2} \exp\left(\frac{r^2(x, y)}{4(t_2 - t_1)}\right).$$

Since

$$H(x, x, t_1) \sim (4\pi t_1)^{-n/2}$$

as $t_1 \to 0$ the estimate of $H(x, y, t)$ follows. To prove the estimate of the theta function, we simply integrate $H(x, x, t)$ over M.

§3. Upper bounds of fundamental solutions

In this section, we will derive upper estimates of any positive L^2 fundamental solution of the equation

$$\left(\Delta - q - \frac{\partial}{\partial t}\right) u(x, t) = 0,$$

where we will assume the potential function q is C^2 and is a function on M alone. We recall again the definitions of ϱ's, since q is time-independent, they can be written as

$$\varrho_{\alpha, R}(x, y, t) = \inf_{\gamma \in \Gamma(R)} \left\{\frac{\alpha}{4t} \int_0^1 |\dot{\gamma}|^2 \, ds + t \int_0^1 q(\gamma(s)) \, ds\right\} \tag{3.1}$$

where $\Gamma(R) = \{\gamma : [0, 1] \to B_p(R) | \gamma(0) = y, \gamma(1) = x\}$. Moreover

$$\varrho_{\alpha, \infty}(x, y, t) = \varrho_\alpha(x, y, t), \tag{3.2}$$

where $\Gamma(\infty) = M$, and

$$\varrho_{1, \infty}(x, y, t) = \varrho_1(x, y, t) = \varrho(x, y, t). \tag{3.3}$$

We remark that when $q \geqslant 0$, ϱ is a metric on M, though ϱ might not be a distance function. Abusing this term, we will refer to ϱ as "the metric" even when q is sometimes not assumed to be nonnegative. The following discussion of ϱ is classical, especially among physicists, hence details of proofs will be omitted.

If γ is a minimizing curve for $\varrho(x, y, t)$, considering a compact perturbation of γ, one computes that the geodesic equation of ϱ is given by

$$\nabla_{\dot{\gamma}} \dot{\gamma} = 2t^2 \nabla q. \tag{3.4}$$

Taking the inner product with $\dot{\gamma}$, (3.4) gives

$$\frac{d}{ds}(|\dot{\gamma}|^2) = 2\langle \nabla_{\dot{\gamma}}\dot{\gamma}, \dot{\gamma}\rangle = 4t^2\langle \nabla q, \dot{\gamma}\rangle.$$

Integrating along γ from 0 to s, we have

$$|\dot{\gamma}|^2(s) - |\dot{\gamma}|^2(0) = 4t^2(q(\gamma(s)) - q(\gamma(0))).$$

Hence

$$|\dot{\gamma}|^2(s) - 4t^2 q(\gamma(s)) = |\dot{\gamma}|^2(0) - 4t^2 q(\gamma(0)), \qquad (3.5)$$

for all $s \in [0, 1]$. If x is not a "cut-point" of y, we can find a 1-parameter family of curves γ_τ, joining $\sigma(\tau)$ to y, where $\sigma: (-\varepsilon, \varepsilon) \to M$ such that $\sigma(0) = x$. We compute

$$\frac{d}{d\tau}\varrho\Big|_{\tau=0} = \frac{1}{2t}\int_0^1 \left\langle \dot{\gamma}, \frac{d}{d\tau}\dot{\gamma}\right\rangle\Big|_{\tau=0} + t\int_0^1 \left\langle \nabla q, \frac{d\gamma}{d\tau}\right\rangle\Big|_{\tau=0}$$

$$= \frac{1}{2t}\left\langle \dot{\gamma}(1), \frac{d\gamma}{d\tau}(1)\right\rangle\Big|_{\tau=0} - \frac{1}{2t}\int_0^1 \left\langle \nabla_{\dot{\gamma}}\dot{\gamma}, \frac{d\gamma}{d\tau}\right\rangle\Big|_{\tau=0} + t\int_0^1 \left\langle \nabla q, \frac{d\gamma}{d\tau}\right\rangle\Big|_{\tau=0}$$

$$= \frac{1}{2t}\left\langle \dot{\gamma}(1), \frac{d\gamma(1)}{d\tau}\right\rangle\Big|_{\tau=0},$$

after using (3.4). We conclude that

$$\nabla_x\varrho(x, y, t) = \frac{1}{2t}\dot{\gamma}(1) \qquad (3.6)$$

and

$$|\nabla_x\varrho|^2(x, y, t) = \frac{1}{4t^2}|\dot{\gamma}|^2(1).$$

Similarly, we compute

$$\frac{\partial\varrho}{\partial t}(x, y, t) = \frac{\partial}{\partial t}\left[\frac{1}{4t}\int_0^1 |\dot{\gamma}|^2 + t\int_0^1 q(\gamma)\right]$$

$$= -\frac{1}{4t^2}\int_0^1 |\dot{\gamma}|^2 + \frac{1}{2t}\int_0^1 \left\langle \dot{\gamma}, \frac{d}{dt}\dot{\gamma}\right\rangle + \int_0^1 q + t\int_0^1 \nabla q \cdot \frac{d\gamma}{dt}$$

$$= -\frac{1}{4t^2}\int_0^1 |\dot{\gamma}|^2 + \int_0^1 q(\gamma),$$

where we have used (3.4), and the assumption that $\gamma_t(0) = y$, and $\gamma_t(1) = x$, for all t.

However, by (3.5), we derive

$$\frac{\partial \varrho}{\partial t}(x, y, t) = -\frac{1}{4t^2} |\dot{\gamma}|^2(1) + q(x).$$

Together with (3.6), we have proved the following:

LEMMA 3.1.

$$|\nabla_x \varrho|^2(x, y, t) + \frac{\partial \varrho}{\partial t}(x, y, t) = q(x)$$

and

$$|\nabla_y \varrho|^2(x, y, t) + \frac{\partial \varrho}{\partial t}(x, y, t) = q(y).$$

We remark that it is also well known that the function ϱ is Lipschitz on M (see Appendix). In particular, the above lemma is valid in the weak sense on M.

Let us define the function

$$g(x, y, t) = -2\varrho(x, y, (1+2\delta) T - t) \tag{3.7}$$

for $x, y \in M$ and $0 \leqslant t \leqslant (1+2\delta) T$, where $\delta > 0$. Lemma 3.1 implies that g satisfies

$$\tfrac{1}{2}|\nabla_y g|^2 + g_t - 2q(y) = 0 \tag{3.8}$$

weakly.

When $q \equiv 0$, we may assume $\partial M \neq \varnothing$ but convex. Since in this case $g(x, y, t)$ is just a multiple of the square of the distance function $r(x, y)$, (3.8) is still valid due to the assumption on ∂M being convex.

LEMMA 3.2. *Let M be a complete manifold which can be either compact or noncompact. Suppose $H(x, y, t)$ is the fundamental solution of (1.1) on $M \times M \times [0, \infty)$. If $q \equiv 0$, we may assume $\partial M \neq \varnothing$ but convex, and $H(x, y, t)$ satisfies either the Dirichlet or the Neumann boundary condition on ∂M. Let*

$$F(y, t) = \int_{S_1} H(y, z, t) H(x, z, T) \, dz \tag{3.9}$$

for $x \in M$, $S_1 \subseteq M$, and $0 \leqslant t \leqslant \tau < (1+2\delta) T$. Then for any subset $S_2 \subseteq M$, we have

$$\int_{S_2} F^2(z, \tau) \, dz \leqslant \int_{S_1} H^2(x, z, T) \, dx \sup_{z \in S_1} \exp\left(-2\varrho(x, z, (1+2\delta) T)\right)$$

$$\times \sup_{z \in S_2} \exp\left(2\varrho(x, z, (1+2\delta) T - \tau)\right).$$

In particular, when $q \equiv 0$, and $S_2 = B_x(R)$, we have

$$\int_{B_x(R)} F^2(z, \tau)\, dz \leq \int_{S_1} H^2(x, z, T)\, dz \exp\left(\frac{-r^2(x, S_1)}{2(1+2\delta)\, T}\right) \exp\left(\frac{R^2}{2(1+2\delta)\, T - 2\tau}\right).$$

Proof. Since F satisfies (1.1), we consider

$$0 = 2 \int_0^\tau \int_M \varphi^2(y) \exp(g(x, y, t))\, F(y, t) \left(\Delta_y - \frac{\partial}{\partial t} - q(y)\right) F(y, t), \qquad (3.10)$$

where $\varphi(y) = \varphi(r(x, y))$ is a cut-off function of the distance to x alone such that

$$\varphi(y) = \begin{cases} 1 & \text{on } B_x(k) \\ 0 & \text{outside } B_x(2k), \end{cases}$$

and $|\nabla \varphi| \leq 3/k$. Integrating the right hand side of (3.10) by parts and using the boundary condition on H, we get

$$\begin{aligned} 0 = &-4 \int_0^\tau \int_M \varphi\, e^g F \langle \nabla \varphi, \nabla F \rangle - 2 \int_0^\tau \int_M \varphi^2 e^g F \langle \nabla g, \nabla F \rangle \\ &- 2 \int_0^\tau \int_M \varphi^2 e^g |\nabla F|^2 + \int_0^\tau \int_M \varphi^2 e^g F^2 g_t \\ &- \int_M \varphi^2 e^g F^2 \Big|_{t=\tau} + \int_M \varphi^2 e^g F^2 \Big|_{t=0} - 2 \int_0^\tau \int_M \varphi^2 e^g F^2 q. \end{aligned} \qquad (3.11)$$

By the Schwarz inequality,

$$-2 \int_0^\tau \int_M \varphi^2 e^g F \langle \nabla g, \nabla F \rangle \leq 2 \int_0^\tau \int_M \varphi^2 e^g |\nabla F|^2 + \frac{1}{2} \int_0^\tau \int_M \varphi^2 e^g F^2 |\nabla g|^2.$$

Combining this with (3.8) and (3.10), we deduce that

$$0 \leq -4 \int_0^\tau \int_M \varphi\, e^g F \langle \nabla \varphi, \nabla F \rangle - \int_M \varphi^2 e^g F^2 \Big|_{t=\tau} + \int_M \varphi^2 e^g F^2 \Big|_{t=0}.$$

Letting $k \to \infty$, since $|\nabla \varphi| \leq 3/k$, the first term on the right hand side of the above inequality vanishes by virtue of the fact that its integrand is L^2. Hence,

$$\int_M \exp(g(x, y, \tau))\, F^2(y, \tau)\, dy \leq \int_M \exp(g(x, y, 0))\, F^2(y, 0)\, dy.$$

Observing that

$$F(y, 0) = \begin{cases} H(x, y, T) & \text{if } y \in S_1 \\ 0 & \text{if } y \notin S_1, \end{cases}$$

and (3.7),

$$\int_M \exp\left(g(x, y, 0)\right) F^2(y, 0) \, dy \leq \sup_{z \in S_1} \exp\left(-2\varrho(x, z, (1+2\delta) T)\right) \int_{S_1} H^2(x, z, T) \, dz.$$

On the other hand,

$$\int_M \exp\left(g(x, y, \tau)\right) F^2(y, \tau) \, dy$$

$$\geq \int_{S_2} \exp\left(g(x, y, \tau)\right) F^2(y, \tau) \, dy$$

$$\geq \inf_{z \in S_2} \exp\left(-2\varrho(x, z, (1+2\delta) T - \tau)\right) \int_{S_2} F^2(y, \tau) \, dy.$$

This proves the lemma.

It is now convenient for us to introduce the following notations: We define

$$\bar{\varrho}_\alpha(x, S, t) = \sup_{z \in S} \varrho_\alpha(x, z, t)$$

and

$$\underline{\varrho}_\alpha(x, S, t) = \inf_{z \in S} \varrho_\alpha(x, z, t)$$

for any subset $S \subseteq M$.

THEOREM 3.1. *Let M be a complete manifold without boundary. Assume the Ricci curvature of M is bounded from below by $-K$, for some constant $K \geq 0$. We also assume that there exists a point $p \in M$, a constant θ, and a function $\gamma(r)$, such that*

$$|\nabla q|(x) \leq \gamma(r(p, x))$$

and

$$\Delta q \leq \theta$$

on M. Then for $x, y \in M$ and $t \in (0, \infty)$, the following estimates are valid:

(i) *If $K=0$, and*

$$\lim_{r \to \infty} \frac{\gamma(r)}{r} = \tau,$$

then

$$H(x, y, t) \leq (1+\delta)^n V^{-1/2}(S_1)\, V^{-1/2}(S_2) \exp\left(C_5(\tau^{2/3}+\theta^{1/2})\,\delta(1+\delta)\,t\right)$$

$$\times \exp\left(2\bar{\varrho}(x, S_2, \delta(1+\delta)\,t)\right) \exp\left(\bar{\varrho}(y, S_1, \delta t)\right)$$

$$\times \exp\left(-\varrho(x, S_1, (1+2\delta)(1+\delta)\,t)\right)$$

for any $\delta>0$, and any subsets S_1, $S_2 \subseteq M$ whose volumes $V(S_1)$ and $V(S_2)$ are finite.
  (ii) If $\gamma(r) \leq \gamma_0$, for some constant γ_0, then

$$H(x, y, t) \leq (1+\delta)^{n\alpha} V^{-1/2}(S_1)\, V^{-1/2}(S_2) \exp\left[C_6(\gamma_0^{2/3}+\theta^{1/2}+(\alpha-1)^{-1}K)\,\delta(2+\delta)\,t\right.$$

$$+\bar{\varrho}_\alpha(x, S_2, \delta(1+\delta)\,t)+\bar{\varrho}_\alpha(y, S_1, \delta t)+\bar{\varrho}(x, S_2, \delta(1+\delta)\,t)$$

$$\left.-\varrho(x, S_1, (1+2\delta)(1+\delta)\,t)\right],$$

for any $\alpha \in (1, 2)$, $\delta>0$, and any subsets S_1, $S_2 \subseteq M$ with finite volumes.

Proof. We will only prove (i), while the proof of (ii) follows similarly by using Corollary 2.3 instead of Corollary 2.2.

To prove (i), we apply Theorem 2.2 to the function $F(y, t)$ of Lemma 3.2. This yields

$$\left(\int_{S_1} H^2(x, z, T)\,dz\right)^2 = F^2(x, T)$$

$$\leq (1+\delta)^n \exp\left[2C_5(\tau^{2/3}+\theta^{1/2})\,\delta T+2\bar{\varrho}(x, S_2, \delta T)\right.$$

$$\left.+2\bar{\varrho}(x, S_2, \delta T)-2\varrho(x, S_1(1+2\delta)\,T)\right] \int_{S_1} H^2(x, z, T)\,dz\, V^{-1}(S_2),$$

by setting $\tau=(1+\delta)\,T$ in Lemma 3.2. Applying Theorem 2.2 to the function $H(x, z, T)$ and setting $T=(1+\delta)\,t$, we obtain

$$H^2(x, y, t) \leq (1+\delta)^{2n} \exp\left[2C_5(\tau^{2/3}+\theta^{1/2})\,\delta(2+\delta)\,t\right.$$

$$+4\bar{\varrho}(x, S_2, \delta(1+\delta)\,t)+2\bar{\varrho}(x, S_1, \delta t)$$

$$\left.-2\varrho(x, S_1, (1+2\delta)(1+\delta)\,t)\right] V^{-1}(S_1)\, V^{-1}(S_2).$$

The theorem follows by taking square root of both sides.

COROLLARY 3.1. *Let M be a complete manifold without boundary. If the Ricci curvature of M is bounded from below by $-K$, for some constant $K \geq 0$, then for $1<\alpha<2$*

and $0<\varepsilon<1$, *the heat kernel satisfies*

$$H(x, y, t) \leqslant C(\varepsilon)^{\alpha} V^{-1/2}(B_x(\sqrt{t}))V^{-1/2}(B_y(\sqrt{t})) \exp\left[C_7 \varepsilon(\alpha-1)^{-1}Kt - \frac{r^2(x,y)}{(4+\varepsilon)t}\right].$$

The constant C_7 depends only on n, while $C(\varepsilon)$ depends on ε with $C(\varepsilon) \to \infty$ as $\varepsilon \to 0$. When $K=0$, the above estimate, after letting $\alpha \to 1$, can be written as

$$H(x, y, t) \leqslant C(\varepsilon) V^{-1}(B_x(\sqrt{t})) \exp\left[\frac{-r^2(x,y)}{(4+\varepsilon)t}\right].$$

Proof. Setting $\gamma_0 = \theta = 0$, $S_1 = B_y(\sqrt{t})$, and $S_2 = B_x(\sqrt{t})$ in the estimate of Theorem 3.1 (ii), we have

$$H(x, y, t) \leqslant (1+\delta)^{n\alpha} V^{-1/2}(B_x(\sqrt{t})) V^{-1/2}(B_y(\sqrt{t}))$$

$$\times \exp[C_6(\alpha-1)^{-1}K\delta(2+\delta)t + 2\bar{\varrho}_{\alpha}(x, B_x(\sqrt{t}), \delta(2+\delta)t)$$

$$+ \bar{\varrho}_{\alpha}(y, B_y(\sqrt{t}), \delta t) - \underline{\varrho}(x, B_y(\sqrt{t}), (1+2\delta)(1+\delta)t)].$$

Since $q \equiv 0$.

$$2\bar{\varrho}_{\alpha}(x, B_x(\sqrt{t}), \delta(2+\delta)t) = \sup_{z \in B_x(\sqrt{t})} \frac{\alpha r^2(x, z)}{2\delta(2+\delta)t} = \frac{\alpha}{2\delta(2+\delta)}. \tag{3.12}$$

Similarly

$$\bar{\varrho}_{\alpha}(y, B_y(\sqrt{t}), \delta t) = \frac{\alpha}{4\delta} \tag{3.13}$$

and

$$\underline{\varrho}(x, B_y(\sqrt{t}), (1+2\delta)(1+\delta)t) = \inf_{z \in B_y(\sqrt{t})} \frac{r^2(x, z)}{4(1+2\delta)(1+\delta)t}. \tag{3.14}$$

If $x \in B_y(\sqrt{t})$, then

$$\underline{\varrho}(x, B_y(\sqrt{t}), (1+2\delta)(1+\delta)t) = 0 \geqslant \frac{r^2(x, y)}{4t} - \frac{1}{4}. \tag{3.15}$$

On the other hand, if $x \notin B_y(\sqrt{t})$, i.e. $r(x, y) > \sqrt{t}$, we have

$$\underline{\varrho}(x, B_y(\sqrt{t}), (1+2\delta)(1+\delta)t) = \frac{(r(x, y)-\sqrt{t})^2}{4(1+2\delta)(1+\delta)t}. \tag{3.16}$$

Applying the inequality

$$(r(x,y)-\sqrt{t})^2 \geq \frac{r^2(x,y)}{1+\delta} - \frac{t}{\delta},$$

and setting $4(1+2\delta)(1+\delta)^2 = 4+\varepsilon$, (3.16) becomes

$$\varrho(x, B_y(\sqrt{t})), (1+2\delta)(1+\delta)t) \geq \frac{r^2(x,y)}{(4+\varepsilon)t} - \frac{1+\delta}{4\varepsilon\delta}.$$

In any case, this together with (3.12), (3.13), and (3.15), proves the first estimate as claimed. To show the second estimate, we apply a volume comparison theorem (see [5]), which states that if $0<R_1<R_2<R_3$, then

$$\frac{V(B_x(R_2))}{V(B_x(R_1))} \leq \frac{V(K,R_2)}{V(K,R_1)} \tag{3.17}$$

and

$$\frac{V(B_x(R_3)-B_x(R_2))}{V(B_x(R_1))} \leq \frac{V(K,R_3)-V(K,R_2)}{V(K,R_1)},$$

where $V(K,R)$ is the volume of the geodesic ball of radius R in the constant $-K/(n-1)$ sectional curvature space form.

To estimate $V(B_x(\sqrt{t}))$ by $V(B_y(\sqrt{t}))$, we consider the following cases:

(a) If $\sqrt{t} > 2r(x,y)$, then

$$V(B_x(\sqrt{t})) \leq V(B_x(\sqrt{t}-r(x,y))) \frac{V(0,\sqrt{t})}{V(0,\sqrt{t}-r(x,y))}$$

$$\leq V(B_y(\sqrt{t})) \left(\frac{\sqrt{t}}{\sqrt{t}-r(x,y)}\right)^n$$

$$\leq 2^{n/2} V(B_y(\sqrt{t})).$$

(b) If $\sqrt{t} \leq 2r(x,y)$, then

$$V(B_x(\sqrt{t})) \leq V(B_x(\sqrt{t}/4)) \frac{V(0,\sqrt{t})}{V(0,\sqrt{t}/4)}$$

$$\leq V(B_y(r(x,y)+\sqrt{t}/4))(4^n)$$

$$\leq 4^n V(B_y(\sqrt{t}/4)) \frac{V(0, r(x,y)+\sqrt{t}/4)}{V(0,\sqrt{t}/4)}$$

$$\leq 4^n V(B_y(\sqrt{t})) \left(\frac{4r(x,y)+\sqrt{t}}{\sqrt{t}}\right)^n.$$

Hence

$$H(x, y, t) \le C(\varepsilon) V^{-1}(B_x(\sqrt{t})) \left(4\frac{r(x, y)}{\sqrt{t}} + 1 \right)^n \exp\left(\frac{-r^2(x, y)}{(4+\varepsilon)t} \right)$$

$$\le C(\varepsilon) V^{-1}(B_x(\sqrt{t})) \exp\left(\frac{-r^2(x, y)}{(4+2\varepsilon)t} \right),$$

by readjusting the constant $C(\varepsilon)$. Now setting $4+2\varepsilon$ to be $4+\varepsilon$, we also derive our estimate as claimed.

It is by now clear that the following theorems follow in exactly the same manner as Theorem 3.1 and Corollary 3.1. Of course, in each case, one uses Theorems 2.3 or 2.1 instead.

THEOREM 3.2. *Let M be a compact manifold with Ricci curvature bounded from below by $-K$, for some constant $K \ge 0$. We assume that the boundary of M is convex, i.e. $\text{II} \ge 0$. Then the fundamental solution $H(x, y, t)$ of the heat equation*

$$\left(\Delta - \frac{\partial}{\partial t} \right) u(x, t) = 0$$

with Neumann boundary condition

$$\frac{\partial u}{\partial v} = 0,$$

must satisfy

$$H(x, y, t) \le C(\varepsilon)^\alpha V^{-1/2}(B_x(\sqrt{t})) V^{-1/2}(B_y(\sqrt{t})) \exp\left[C_7 \varepsilon(\alpha-1)^{-1} Kt - \frac{r^2(x, y)}{(4+\varepsilon)t} \right]$$

for all $1 < \alpha < 2$ and $0 < \varepsilon < 1$, where the constant $C(\varepsilon) \to \infty$ as $\varepsilon \to 0$. When $K=0$, after letting $\alpha \to 1$, this estimate can be written as

$$H(x, y, t) \le C(\varepsilon) V^{-1}(B_x(\sqrt{t})) \exp\left(\frac{-r^2(x, y)}{(4+\varepsilon)t} \right).$$

THEOREM 3.3. *Let M be a complete manifold without boundary. Assume $p \in M$ and let $B_p(2R)$ be the geodesic ball of radius $2R$ centered at p. We denote $-K(2R)$, with $K(2R) \ge 0$, by a lower bound of the Ricci curvature on $B_p(2R)$. We also assume that q is a C^2 function on M with*

$$\Delta q \le \theta(2R)$$

and

$$|\nabla q| \leqslant \gamma(2R)$$

on $B_p(2R)$. *Then for any $a>1$, x, $y \in B_p(R)$, S_1 and S_2 any subsets of $B_p(R)$, a fundamental solution $H(x, y, t)$ of the equation*

$$\left(\Delta - q - \frac{\partial}{\partial t}\right) u(x, t) = 0$$

must satisfy

$$H(x, y, t) \leqslant (1+\delta)^n V^{-1/2}(S_1)\, V^{-1/2}(S_2) \exp(A\delta(2+\delta)\, t)$$

$$\times \exp[\bar{\varrho}_{\alpha, R}(x, S_2, \delta(1+\delta)\, t) + \bar{\varrho}_{\alpha, R}(y, S_1, \delta t)$$

$$- \underline{\varrho}(x, S_1, (1+2\delta)(1+\delta)\, t) + \bar{\varrho}(x, S_2, \delta(1+\delta)\, t)]$$

where

$$A = C_7[aR^{-1}\sqrt{\bar{K}} + a^3(\alpha-1)^{-1}R^{-2} + \gamma^{2/3}(\alpha-1)^{1/3}\alpha^{-1/3} + (\alpha\theta)^{1/2} + \alpha(\alpha-1)^{-1}K].$$

The estimate given by Theorem 3.1 can be written in a more comprehensible form when the potential is nonnegative. In fact in this case, we see that

$$\varrho(x, y, t) \geqslant \frac{r^2(x, y)}{4t}.$$

This ensures that $\varrho(x, y, t)$ is a proper function in the y-variable.

COROLLARY 3.2. *Let M and q satisfy the hypothesis of Theorem 3.1. We also assume that q is nonnegative. The following estimates hold:*

If (i) *of Theorem 3.1 is valid, then for all $a>0$,*

$$H(x, y, t) \leqslant C^a(\varepsilon)\, V^{-1/2}(S_a(x, t))\, V^{-1/2}(S_a(y, t))$$

$$\times \exp\left[C_5\, \varepsilon(\tau^{2/3} + \theta^{1/2})\, t - (1+\varepsilon)^{-1}\varrho(x, y, t)\right],$$

for all $0<\varepsilon<\frac{1}{2}$.

If (ii) *of Theorem 3.1 is valid, then*

$$H(x, y, t) \leqslant C(\varepsilon)^{aa} V^{-1/2}(S_a(x, t))\, V^{-1/2}(S_a(y, t))$$

$$\times \exp\left[C_6(\gamma_0^{2/3} + \theta^{1/2} + (\alpha-1)^{-1}K)\, t - (1+\varepsilon)^{-1}\varrho(x, y, t)\right],$$

for all $0<\varepsilon<\frac{1}{2}$ and $1\leqslant\alpha\leqslant2$.

In both cases, $C(\varepsilon)$ is a constant depending on n and ε with $C(\varepsilon) \to \infty$ as $\varepsilon \to 0$, and
$S_a(x, t) = \{z \in M | \varrho(x, z, t) \leq a\}$.

Proof. We will only give the proof of (ii), while (i) follows identically. By the nonnegativity of q, we observe that if $t_1 \leq t_2$, then

$$
\begin{aligned}
\varrho_a(x, y, t_1) &= \inf_\gamma \left\{ \frac{a}{4t_1} \int_0^1 |\dot{\gamma}|^2 + t_1 \int_0^1 q \right\} \\
&= \inf_\gamma \left\{ \frac{at_2}{t_1} \left(\frac{1}{4t_2} \int_0^1 |\dot{\gamma}|^2 + t_2 \int_0^1 q \right) - \left(\frac{at_2^2}{t_1} - t_1 \right) \int_0^1 q \right\} \\
&= \inf_\gamma \left\{ \frac{at_2}{t_1} \left(\frac{1}{4t_2} \int_0^1 |\dot{\gamma}|^2 + t_2 \int_0^1 q \right) \right\} \\
&= \frac{at_2}{t_1} \varrho(x, y, t_2),
\end{aligned}
\tag{3.18}
$$

for all $\alpha \geq 1$. By Theorem 3.1 (ii), if we set $S_1 = S_a(y, t)$ and $S_2 = S_a(x, t)$, we only need to estimate the following:

$$
\bar{\varrho}_a(x, S_a(x, t), \delta(1 + \delta) t) \leq \frac{\alpha}{\delta(1 + \delta)} \bar{\varrho}(x, S_a(x, t), t) \leq \frac{\alpha a}{\delta(1 + \delta)},
$$

and similarly

$$
\bar{\varrho}_a(y, S_a(y, t), \delta t) \leq \frac{\alpha a}{\delta},
$$

and

$$
\bar{\varrho}(x, S_a(x, t), \delta(1 + \delta) t) \leq \frac{a}{\delta(1 + \delta)}.
$$

Finally

$$
\underline{\varrho}(x, S_a(y, t), (1 + 2\delta)(1 + \delta) t) \geq \frac{1}{(1 + 2\delta)(1 + \delta)} \underline{\varrho}(x, S_a(y, t), t).
$$

If $x \in S_a(y, t)$, then we observe that

$$
\underline{\varrho}(x, S_a(y, t), t) \geq 0 \geq \varrho(x, y, t) - 1.
$$

On the other hand, if $x \notin S_a(y, t)$, then for any $z \in S_a(y, t)$, we claim that

$$
\varrho(x, z, t) \geq \varrho(x, y, (1 + \varepsilon) t) - \varrho(y, z, \varepsilon t).
\tag{3.19}
$$

Indeed, if γ_1 and γ_2 are the minimizing curves for $\varrho(z, x, t)$ and $\varrho(y, z, t)$ respectively, we reparametrize $\gamma_1 \cup \gamma_2 = \gamma$ defined by

$$
\gamma(s) = \begin{cases} \gamma_1((1+\varepsilon)s), & \text{if } 0 \leqslant s \leqslant \dfrac{1}{1+\varepsilon} \\[2mm] \gamma_2((1+\varepsilon)\varepsilon^{-1}s - \varepsilon^{-1}), & \text{if } \dfrac{1}{1+\varepsilon} \leqslant s \leqslant 1. \end{cases}
$$

Clearly $\gamma(0) = x$ and $\gamma(1) = y$, hence

$$
\begin{aligned}
\varrho(x, y, (1+\varepsilon)t) &\leqslant \frac{1}{4(1+\varepsilon)t} \int_0^1 |\dot{\gamma}|^2 + (1+\varepsilon)t \int_0^1 q(\gamma(s)) \\
&= \frac{1+\varepsilon}{4(1+\varepsilon)t} \int_0^1 |\dot{\gamma}_1|^2 + \frac{(1+\varepsilon)t}{1+\varepsilon} \int_0^1 q(\gamma_1) \\
&\quad + \frac{(1+\varepsilon)\varepsilon^{-1}}{4(1+\varepsilon)t} \int_0^1 |\dot{\gamma}_2|^2 + \frac{(1+\varepsilon)t}{(1+\varepsilon)\varepsilon^{-1}} \int_0^1 q(\gamma_2) \\
&= \varrho(x, z, t) + \varrho(y, z, \varepsilon t).
\end{aligned}
$$

Therefore (3.19) is valid. To conclude the proof, we simply apply (3.18) again and deduce that

$$
\begin{aligned}
\varrho(x, z, t) &\geqslant (1+\varepsilon)^{-1}\varrho(x, y, t) - \varepsilon^{-1}\varrho(y, z, t) \\
&\geqslant (1+\varepsilon)^{-1}\varrho(x, y, t) - \varepsilon^{-1}a,
\end{aligned}
$$

for all $z \in S_a(y, t)$.

§4. Lower bounds of fundamental solutions

The goal of this section is to derive lower estimates on positive fundamental solutions of the equation

$$
\left(\Delta - q - \frac{\partial}{\partial t} \right) u(x, t) = 0,
$$

where q is a C^2 function on M.

When $q \equiv 0$, Cheeger–Yau [6] proved a lower estimate of the heat kernel in terms of the kernel of a model. In particular, they showed that if the Ricci curvature of M is bounded from below by $-K$ with $K \geqslant 0$, then the heat kernel of M is bounded from below by the heat kernel of the constant curvature simply connected space form with

sectional curvature identically $-(n-1)^{-1}K$. In Theorem 4.1 below, we will prove an estimate which is different from that of Cheeger–Yau. When $K=0$, this estimate which we will derive is sharp in order, especially for large t. However, when $K>0$, our estimate does not seem sharper than that in [6]. In view of this, we will only prove the theorem for $K=0$.

THEOREM 4.1. *Let M be a complete manifold without boundary. Suppose the Ricci curvature of M is nonnegative. Then the fundamental solution of the heat equation satisfies*

$$H(x, y, t) \geq C^{-1}(\varepsilon) \, V^{-1}(B_x(\sqrt{t})) \exp\left(\frac{-r^2(x, y)}{(4-\varepsilon)t}\right)$$

where $C(\varepsilon)$ depends on $\varepsilon>0$ and n with $C(\varepsilon) \to \infty$ as $\varepsilon \to 0$. Symmetrizing the above estimate, we also have

$$H(x, y, t) \geq C^{-1}(\varepsilon) \, V^{-1/2}(B_x(\sqrt{t})) \, V^{-1/2}(B_y(\sqrt{t})) \exp\left(\frac{-r^2(x, y)}{(4-\varepsilon)t}\right).$$

Proof. By Theorem 2.2, we have

$$\int_{B_x(R)} H(z, y, (1-\delta)t) \leq V(B_x(R)) \, H(x, y, t)(1-\delta)^{-n/2} \exp\left(\frac{r^2}{4\delta t}\right). \qquad (4.1)$$

We will estimate the left hand side of (4.1). Let the function $\varphi(z)$ be defined as $\varphi(z)=\varphi(r(x, z))$ which is a function of $r(x, z)$ with

$$\varphi(r(x, z)) = \begin{cases} 1 & \text{on } B_x(\sqrt{1-\delta}\,R) \\ 0 & \text{outside } B_x(R), \end{cases}$$

$0 \leq \varphi \leq 1$, and $\partial\varphi/\partial r < 0$. If we let

$$F(y, t) = \int_M \varphi(r(x, z)) \, H(z, y, t)$$

be the solution of the heat equation with $\varphi(r(x, y))$ as initial condition, then

$$\int_{B_x(R)} H(z, y, t) \geq F(y, t).$$

To estimate $F(y, t)$ from below, we apply the method of Cheeger and Yau in [6]. We will simply outline the argument as follows:

Let $\bar{F}(r, t)$ be the solution of the heat equation in $\mathbf{R}^n$ with initial data

$$\bar{F}(r, 0) = \varphi(r),$$

where r is the distance to the origin. Since φ is a function of the distance alone, one verifies that $\bar{F}$ must also be a function of r for any fixed time. Hence, the notation $\bar{F}(r, t)$ is valid. By the argument in [6], we conclude that

$$\bar{F}(r(x, y), t) \leq F(y, t), \tag{4.2}$$

provided we can justify the assumption

$$\frac{\partial \bar{F}}{\partial r}(r, t) \leq 0$$

on $\mathbf{R}^n \times [0, \infty)$. However, by rotational symmetry of $\bar{F}$, we see that

$$\frac{\partial \bar{F}}{\partial r}(0, t) = 0 \tag{4.3}$$

for all t. Also

$$\frac{\partial \bar{F}}{\partial r}(r, 0) = \frac{\partial \varphi}{\partial r} \leq 0, \tag{4.4}$$

and

$$\lim_{r \to \infty} \frac{\partial \bar{F}}{\partial r}(r, t) = 0. \tag{4.5}$$

for all t, since φ' has compact support. Moreover $\partial F/\partial r$ satisfies the differential equation

$$\left[\frac{\partial^2}{\partial r^2} + (n-1) r^{-1} \frac{\partial}{\partial r} - (n-1) r^{-2} - \frac{\partial}{\partial t} \right] \frac{\partial \bar{F}}{\partial r} = 0.$$

Applying the maximum principle for parabolic equations on $[0, \infty) \times [0, \infty)$, and in view of the boundary conditions (4.3), (4.4), and (4.5), we conclude that

$$\frac{\partial \bar{F}}{\partial r} \leq 0.$$

Therefore, (4.2) is valid. Hence

$$F(y, t) \geq (4\pi t)^{-n/2} \int_{\mathbf{R}^n} \varphi(|\bar{z}|) \exp\left(\frac{-|\bar{y} - \bar{z}|^2}{4t} \right) d\bar{z},$$

with $|\bar{y}| = r(x, y)$. Combining with (4.1) and setting $R = \sqrt{t}$, we have

$$H(x, y, t) \geq C(\delta) V(B_x(\sqrt{t})) t^{-n/2} \int_{|\bar{z}| \leq \sqrt{(1-\delta)t}} \exp\left(\frac{-|\bar{y}-\bar{z}|^2}{4(1-\delta)t}\right) d\bar{z}$$

$$\geq C(\delta) V(B_x(\sqrt{t})) \exp\left(\frac{-|\bar{y}|^2}{4(1-\delta)t}\right).$$

Writing $4 - \varepsilon = 4(1 - \delta)$, the theorem follows.

THEOREM 4.2. *Let M be a compact manifold with boundary, ∂M. Suppose the Ricci curvature of M is nonnegative, and if $\partial M \neq \varnothing$, we assume that ∂M is convex, i.e. $\mathrm{II} \geq 0$. Then the fundamental solution of the heat equation with Neumann boundary condition satisfies*

$$H(x, y, t) \geq C^{-1}(\varepsilon) V^{-1}(B_x(\sqrt{t})) \exp\left(\frac{-r^2(x, y)}{(4-\varepsilon)t}\right)$$

for some constant $C(\varepsilon)$ depending on $\varepsilon > 0$ and n such that $C(\varepsilon) \to \infty$ as $\varepsilon \to 0$. Moreover, by symmetrizing,

$$H(x, y, t) \geq C^{-1}(\varepsilon) V^{-1/2}(B_x(\sqrt{t})) V^{-1/2}(B_y(\sqrt{t})) \exp\left(\frac{-r^2(x, y)}{(4-\varepsilon)t}\right).$$

Proof. We can apply Theorem 2.3 to obtain (4.1). Following the notation as in Theorem 4.1, we only need to show that

$$F(y, t) \geq \bar{F}(r(x, y), t).$$

Their difference,

$$G(y, t) = F(y, t) - \bar{F}(r(x, y), t),$$

satisfies the inequality

$$\left(\Delta - \frac{\partial}{\partial t}\right) G(y, t) \leq 0,$$

in the sense of distributions. We now claim that

$$\frac{\partial G}{\partial \nu}(y, t) \geq 0 \tag{4.6}$$

weakly on ∂M for a dense subset of $x \in M$. Clearly, to prove the estimate of $H(x, y, t)$, it suffices to prove it on a dense subset of $x \in M$. The general case will follow by passing to the limit.

Assume (4.6) holds for a particular $x \in M$. To show that $G(y, t) \geq 0$, we simply consider the function

$$G_-(y, t) = \begin{cases} G(y, t), & \text{if } G(y, t) \leq 0 \\ 0, & \text{if } G(y, t) \geq 0. \end{cases}$$

$G_-(y, t)$ is a Lipschitz function on M and it is nonpositive. Hence

$$\int_0^T \int_M G_-(y, t) \Delta G(y, t) \, dy \, dt = \int_0^T \int_M G_-(y, t) \frac{\partial G}{\partial t}(y, t) \, dy \, dt. \tag{4.7}$$

The left hand side of (4.7) can be written as

$$\int_0^T \int_M G_-(y, t) \frac{\partial G_-}{\partial t}(y, t) \, dy \, dt = \frac{1}{2} \int_0^T \frac{\partial}{\partial t} \int_M G_-^2(y, t) \, dy \, dt$$

$$= \frac{1}{2} \int_M G_-^2(y, T) \, dy - \frac{1}{2} \int_M G_-^2(y, 0) \, dy$$

$$= \frac{1}{2} \int_M G_-^2(y, T) \, dy.$$

The last equality follows from the fact that $G(y, 0) = 0$. On the other hand, the right hand side of (4.7) can be calculated as follows:

$$\int_0^T \int_M G_-(y, t) \Delta G(y, t) \, dy \, dt = -\int_0^T \int_M \langle \nabla G_-(y, t), \nabla G(y, t) \rangle \, dy \, dt$$

$$+ \int_0^T \int_M G_-(y, t) \frac{\partial G}{\partial \nu}(y, t) \, dy \, dt$$

$$\leq -\int_0^T \int_M |\nabla G_-(y, t)|^2 \, dy \, dt.$$

Hence, we have

$$-\int_0^T \int_M |\nabla G_-(y, t)|^2 \, dy \, dt \geq \frac{1}{2} \int_M G_-^2(y, T) \, dy.$$

Therefore $G(y, T) \geq 0$, and since T is arbitrary, this proves the required inequality. The estimate for such a point x will follow from the rest of the argument in Theorem 4.1.

To prove the claim that for a dense subset of $x \in M$, (4.6) holds weakly, we observe that since $\bar{F}$ is a decreasing function of $r(x, y)$, it suffices to show that

$$\frac{\partial r(x, y)}{\partial \nu} \geq 0 \tag{4.8}$$

weakly for a dense set of $x \in M$. With this flexibility of slight perturbation of x, we may assume that the cut-locus of x intersects ∂M along a set with $(n-1)$-measure zero. We denote this set by $\mathscr{S} \subseteq \partial M$. For any $y \in \partial M - \mathscr{S}$, there exists a unique geodesic $\gamma(s)$ joining x to y with $\gamma(0) = x$ and $\gamma(r(x, y)) = y$. This geodesic is the distance realizing curve because ∂M is convex. Clearly

$$\frac{\partial r(x, y)}{\partial \nu} = \frac{\partial r(\gamma(s), y)}{\partial \nu},$$

for all $s \in [0, r(x, y)]$. On the other hand, by the convexity of ∂M,

$$\frac{\partial r(\gamma(s), y)}{\partial \nu} \geqslant 0$$

for s sufficiently close to $r(x, y)$. Hence inequality (4.8) is established for $y \notin \mathscr{S}$ which was claimed.

We will now prove a lower bound for the fundamental solution of the equation

$$\left(\Delta - q - \frac{\partial}{\partial t} \right) u(x, t) = 0.$$

Similar to the upper bound obtained in §3, we have to assume that M has Ricci curvature bounded from below by 0 and Δq is bounded from above.

THEOREM 4.3. *Let M be complete manifold without boundary. Assume that the Ricci curvature of M is nonnegative. Suppose q is a C^2 function on M with*

$$\Delta q \leqslant \theta$$

and

$$\exp(-\varrho(x, y, t)) \in L^2(M).$$

Then the fundamental solution, $H(x, y, t)$, of the equation

$$\left(\Delta - q - \frac{\partial}{\partial t} \right) u(x, t) = 0,$$

must satisfy

$$H(x, y, t) \geqslant (4\pi t)^{-n/2} \exp\left(-\left(\frac{n\theta}{2} \right)^{1/2} t - \varrho(x, y, t) \right).$$

Proof. We will first study the "geodesics" corresponding to the metric $\varrho(x, y, t)$. To do this, we assume that x is not a cut point of y, that is, for any point z in a

neighborhood of x, there exists a unique distance minimizing curve γ which gives

$$\varrho(x, z, t) = \frac{1}{4t} \int_0^1 |\dot{\gamma}|^2 + t \int_0^1 q(\gamma(s)).$$

All the theories which we will derive for the metric $\varrho(x, y, t)$ are parallel to the Riemannian situation $(q=0)$. Hence, we will only outline the proofs, and the reader can consult [3] for a more detailed line by line explanation.

We recall that by the first variation formula for geodesics, we have the geodesic equation given by (3.4), i.e.

$$\nabla_{\dot{\gamma}} \dot{\gamma} = 2t^2 \nabla q \tag{4.9}$$

and

$$\nabla_x \varrho(x, y, t) = \frac{1}{2t} \dot{\gamma}(1). \tag{4.10}$$

The second variation formula for geodesics is given by

$$
\begin{aligned}
\frac{\partial^2 \varrho}{\partial v^2}\bigg|_{v=0} &= \frac{1}{2t}\left\{ \int_0^1 \langle \nabla_V \nabla_T V, T \rangle + \int_0^1 \langle \nabla_T V, \nabla_T V \rangle \right\} + t\left\{ \int_0^1 \langle \nabla q, \nabla_V V \rangle + \int_0^1 \langle \nabla_V(\nabla q), V \rangle \right\} \\
&= \frac{1}{2t}\left\{ \int_0^1 \langle R_{TV} T, V \rangle + \int_0^1 \langle \nabla_T \nabla_V V, T \rangle + \int_0^1 |\nabla_T V|^2 \right\} \\
&\quad + t\left\{ \int_0^1 \langle \nabla q, \nabla_V V \rangle + \int_0^1 \langle \nabla_V(\nabla q), V \rangle \right\} \\
&= \frac{1}{2t}\left\{ \int_0^1 \langle R_{TV} T, V \rangle + \int_0^1 T\langle \nabla_V V, T \rangle - \int_0^1 \langle \nabla_V V, \nabla_T T \rangle + \int_0^1 |\nabla_T V|^2 \right\} \\
&\quad + t\left\{ \int_0^1 \langle \nabla q, \nabla_V V \rangle + \int_0^1 \langle \nabla_V(\nabla q), V \rangle \right\}.
\end{aligned}
\tag{4.11}
$$

Using (4.9) with $T=\dot{\gamma}$ and the fact that $\langle \nabla_V(\nabla q), V \rangle = \mathrm{Hess}_q(V, V)$, we have

$$\frac{\partial^2 \varrho}{\partial v^2}\bigg|_{v=0} = \frac{1}{2t}\left\{ \int_0^1 \langle R_{TV} T, V \rangle + \langle \nabla_V V, T \rangle \bigg|_0^1 + \int_0^1 |\nabla_T V|^2 \right\} + t \int_0^1 \mathrm{Hess}_q(V, V).$$

Moreover, by differentiating (4.9), we see that the Jacobi equation is given by

$$\nabla_V \nabla_T T = 2t^2 \nabla_V(\nabla q).$$

But

$$\nabla_V \nabla_T T = \nabla_T \nabla_V T + R_{VT} T,$$

whence we can write the Jacobi equation as

$$\nabla_T \nabla_V T = R_{TV} T + 2t^2 \nabla_V(\nabla q). \tag{4.12}$$

If we fix the point y and compute the second derivative of ϱ as a function of x, then the variational vector field can be taken to satisfy

$$V(0) = 0$$

and

$$\nabla_V V(1) = 0.$$

Then

$$\frac{\partial^2 \varrho}{\partial V^2}\bigg|_{v=0} = \frac{1}{2t}\left\{\int_0^1 \langle R_{TV} T, V \rangle + \int_0^1 |\nabla_T V|^2\right\} + t \int_0^1 \text{Hess}_q(V, V)$$

$$= I(V, V),$$

which is the index form along γ joining y to x. One checks that the basic index form lemma is still valid (see Lemma 1.21 in [3]). In fact, if γ has no conjugate points, i.e. if there are no Jacobi fields vanishing at $\gamma(0)$ and $\gamma(s)$ for all $s \in (0, 1]$, and if V is a Jacobi field along γ, then for any arbitrary vector field W along γ with $W(0) = V(0) = 0$ and $W(1) = V(1)$,

$$I(V, V) \leqslant I(W, W).$$

Up to this point, the function q is completely arbitrary. From now on, we will assume that q satisfies

$$\Delta q \leqslant \theta$$

on M. Moreover, we also assume that M has nonnegative Ricci curvature.

In this case, we consider $e_1, \ldots, e_n$, n parallel orthonormal vector fields along γ. We define $W_i(s) = s^\alpha e_i$ with $|W_i|(1) = 1$. By the second variation formula and the index form lemma,

$$\nabla_y \varrho(x, y, t) \leqslant \sum_{i=1}^n I(W_i, W_i)$$

$$= \frac{1}{2t}\left\{\sum_{i=1}^n \int_0^1 \langle R_{TW_i} T, W_i \rangle + \int_0^1 \sum_{i=1}^n |\nabla_T W_i|^2\right\} + t \int_0^1 \sum_{i=1}^n \text{Hess}_q(W_i, W_i)$$

$$= \frac{1}{2t}\left\{-\int_0^1 S^{2\alpha} \text{Ric}(T, T) + \int_0^1 n\alpha^2 S^{2\alpha-2}\right\} + t \int_0^1 S^{2\alpha} \Delta q$$

$$\leqslant \frac{n\alpha^2}{2t(2\alpha-1)} + \frac{\theta t}{2\alpha+1}$$

$$\leqslant \frac{n}{2t}\left[\frac{\alpha^2}{2\alpha-1} + \frac{2\theta t^2}{n(2\alpha-1)}\right].$$

Choosing $1<\alpha<\infty$ to minimize the right hand side by setting

$$\alpha = \frac{1}{2}\left(1+\sqrt{1+\frac{8t^2\theta}{n}}\right),$$

we have

$$\Delta_y \varrho(x,y,t) \leqslant \frac{n}{2t}\left[\frac{1}{2}\left(1+\sqrt{1+\frac{8t^2\theta}{n}}\right)\right]$$

$$\leqslant \frac{n}{2t}\left[\frac{1}{2}+\frac{1}{2}+t\sqrt{\frac{2\theta}{n}}\right] \tag{4.13}$$

$$= \frac{n}{2t}+\left(\frac{n\theta}{2}\right)^{1/2}.$$

This inequality, as it stands, is only valid when y is not a cut point of x. However, following an argument of [5] and [27], and using the fact that (4.10) implies that the gradient of ϱ points into the cut locus, inequality (4.13) holds on M in the sense of distributions.

To complete the proof of the theorem, we simply compute

$$\left(\Delta-q-\frac{\partial}{\partial t}\right)(4\pi t)^{-n/2}\exp\left(-\left(\frac{n\theta}{2}\right)^{1/2}t-\varrho(x,y,t)\right)$$

$$\geqslant (4\pi t)^{-n/2}\exp\left(-\left(\frac{n\theta}{2}\right)^{1/2}t-\varrho(x,y,t)\right)\left[|\nabla\varrho|^2-\Delta\varrho-q+\frac{n}{2t}+\left(\frac{n\theta}{2}\right)^{1/2}+\varrho_t\right]$$

$$\geqslant 0,$$

in the sense of distributions. Since

$$\lim_{t\to 0}(4\pi t)^{-n/2}\exp\left(-\left(\frac{n\theta}{2}\right)^{1/2}t-\varrho(x,y,t)\right) = \delta_x(y),$$

it follows from the fact that $\exp(-\varrho)$ is in $L^2(M)$ and from Duhamel's principle that

$$H(x,y,t) \geqslant (4\pi t)^{-n/2}\exp\left(-\left(\frac{n\theta}{2}\right)^{1/2}t-\varrho(x,y,t)\right).$$

We point out that the L^2 assumption of $\exp(-\varrho)$ is rather mild. In particular, if q is

bounded from below by a constant q_0, then

$$\exp(-\varrho(x, y, t)) \leq \exp\left(-\frac{r^2(x, y)}{4t} - tq_0\right)$$

which is clearly L^2 on a manifold with nonnegative Ricci curvature.

§5. Heat equation and Green's kernel

We will utilize the Harnack inequality, the upper and lower estimates of the heat kernel to derive some properties of the heat equation and Green's kernel on a complete manifold. Later on, we will also apply our upper bound to obtain estimates on eigenvalues and Betti numbers for compact manifolds.

THEOREM 5.1. *Let M be a complete manifold with Ricci curvature satisfying*

$$\text{Ric}(x) \geq -C_9 r^2(p, x)$$

for some constant, $C_9 > 0$, where $r(p, x)$ denotes the distance from x to some fixed point $p \in M$. Then any solution $u(x, t)$ of the heat equation

$$\left(\Delta - \frac{\partial}{\partial t}\right) u(x, t)$$

on $M \times [0, \infty)$ which is bounded from below is uniquely determined by its initial data $u(x, 0) = u_0(x)$.

Proof. We may assume, by adding a constant to $u(x, t)$, that $u(x, t) \geq 0$. Let us first prove that $u(x, t)$ is uniquely determined when $u_0(x) \equiv 0$. In this case, we will show that $u(x, t) \equiv 0$.

First, we observe that by defining

$$v(x, t) = \begin{cases} 0, & \text{if } 0 \leq t \leq 1 \\ u(x, t-1), & \text{if } t \geq 1 \end{cases}$$

on $M \times [0, \infty)$, $v(x, t)$ is a weak solution of the heat equation

$$\left(\Delta - \frac{\partial}{\partial t}\right) v(x, t) = 0.$$

By regularity, $v(x, t)$ must, in fact, be a smooth solution. Applying the Harnack inequality to $v(x, t)$, we conclude that

$$v(x, t) \leq v(p, t_0) \left(\frac{t_0}{t} \right)^{n\alpha/2} \exp \left(A(t_0 - t) + \frac{\alpha r^2(x, p)}{4(t_0 - t)} \right),$$

where

$$A \leq C_7 [2\alpha C_9^{1/2} + \alpha^3 (\alpha - 1)^{-1} r^{-2}(x, p) + 4\alpha(\alpha - 1)^{-1} C_9 r^2(x, p)].$$

In order to obtain the above estimate of A, we have used the curvature assumption. Setting $\alpha = 2$, and $1 \leq t \leq t_0/2$, we have

$$v(x, t) \leq v(p, t_0) C(t_0) \exp (C(t_0) r^2(x, p))$$

for all $x \in M$. Since $v \equiv 0$ on $M \times [0, 1]$, the above growth estimate is valid on $M \times [0, t_0/2]$. Applying the uniqueness theorem in [15], we conclude that $v \equiv 0$ on $M \times [0, t_0/2]$. However t_0 is arbitrary, this shows that $v \equiv 0$ on $M \times [0, \infty)$, and hence $u \equiv 0$ on $M \times [0, \infty)$, as claimed.

To prove the general case $u_0(x) \geq 0$, we observe that by the maximum principle, the solution $u_k(x, t)$ of the heat equation with initial data

$$u_k(x, 0) = \varphi_k(r(p, x)) u_0(x)$$

satisfies

$$u_k(x, t) \leq u(x, t),$$

if $\varphi_k(r(p, x))$ is a cut-off function with $0 \leq \varphi_k \leq 1$, and

$$\varphi_k(r) = \begin{cases} 1, & \text{if } r \leq k \\ 0, & \text{if } r \geq 2k. \end{cases}$$

We now claim that $u_k(x, t) \to u(x, t)$ uniformly on compact subsets of M. Indeed, since $0 \leq u_k \leq u$, and by the monotonicity of u_k in k, the sequence must converge uniformly on any compact subset to some solution $v(x, t)$ of the heat equation with $v(x, 0) = u_0(x)$. However, $u_k \leq u$, $v \leq u$ on $M \times [0, \infty)$. Applying our uniqueness argument to $u - v$ which is a nonnegative solution with initial data $(u - v)(x, 0) = 0$, we conclude $u_k \to u$ uniformly on compact sets. However, the heat equation is known to preserve $L^2(M)$ and is unique in $L^2(M)$, whence each of the u_k is uniquely determined. Passing to the limit, so is u.

On a complete manifold, one defines the Green's function

$$G(x, y) = \int_0^\infty H(x, y, t) \, dt$$

if the integral on the right hand side converges. One checks readily, that G is positive and $\Delta G(x, y) = -\delta_x(y)$.

THEOREM 5.2. *Let M be a complete manifold with nonnegative Ricci curvature. If $G(x, y)$ exists, then there exist constants C_{10} and C_{11} depending only on n, such that*

$$C_{10} \int_{r^2}^{\infty} V^{-1}(B_x(\sqrt{t}))\, dt \leq G(x, y)$$

$$\leq C_{11} \int_{r^2}^{\infty} V^{-1}(B_x(\sqrt{t}))\, dt$$

and

$$C_{10} \int_{r^2}^{\infty} V^{-1/2}(B_x(\sqrt{t}))\, V^{-1/2}(B_y(\sqrt{t}))\, dt \leq G(x, y)$$

$$\leq C_{11} \int_{r^2}^{\infty} V^{-1/2}(B_x(\sqrt{t}))\, V^{-1/2}(B_y(\sqrt{t}))\, dt$$

where $r = r(x, y)$.

Proof. It suffices to show that

$$\int_0^{r^2} H(x, y, t)\, dt \leq C_{12} \int_{r^2}^{\infty} V^{-1}(B_x(\sqrt{t}))\, dt \tag{5.1}$$

and

$$\int_0^{r^2} H(x, y, t)\, dt \leq C_{12} \int_{r^2}^{\infty} V^{-1/2}(B_x(\sqrt{t}))\, V^{-1/2}(B_y(\sqrt{t}))\, dt. \tag{5.2}$$

Indeed, by Theorem 3.1, we have

$$G(x, y) = \int_0^{\infty} H(x, y, t)\, dt \leq \int_0^{r^2} H(x, y, t)\, dt + \int_{r^2}^{\infty} H(x, y, t)\, dt$$

$$\leq \int_0^{r^2} H(x, y, t)\, dt + C_{10} \int_{r^2}^{\infty} V^{-1}(B_x(\sqrt{t}))\, dt$$

and similarly

$$G(x, y) \leq \int_0^{r^2} H(x, y, t)\, dt + C_{11} \int_{r^2}^{\infty} V^{-1/2}(B_x(\sqrt{t}))\, V^{-1/2}(B_y(\sqrt{t}))\, dt.$$

Moreover, the lower bound of G follows by applying Theorem 4.1 to the inequality

$$G(x, y) \geq \int_{r^2}^{\infty} H(x, y, t) \, dt.$$

To prove (5.1), we apply Theorem 3.1 to get

$$\int_0^{r^2} H(x, y, t) \, dt \leq C_{10} \int_0^{r^2} V^{-1}(B_x(\sqrt{t})) \exp\left(\frac{-r^2}{5t}\right) dt.$$

Letting $s = r^4/t$, where $r^2 \leq s < \infty$, we have

$$\int_0^{r^2} V^{-1}(B_x(\sqrt{t})) \exp\left(\frac{-r^2}{5t}\right) dt = \int_{r^2}^{\infty} V^{-1}\left(B_x\left(\frac{r^2}{\sqrt{s}}\right)\right) \exp\left(\frac{-s}{5r^2}\right) \frac{r^4}{s^2} \, ds. \quad (5.3)$$

On the other hand, the comparison theorem (3.17) yields

$$V\left(B_x\left(\frac{r^2}{\sqrt{s}}\right)\right) \geq V(B_x(\sqrt{s})) \frac{V\left(0, \frac{r^2}{\sqrt{s}}\right)}{V(0, \sqrt{s})} = V(B_x(\sqrt{s}))\left(\frac{r^2}{s}\right)^n.$$

Hence (5.3) becomes

$$\int_0^{r^2} H(x, y, t) \, dt \leq C_{10} \int_{r^2}^{\infty} V^{-1}\left(B_x(\sqrt{s})\right)\left(\frac{r^2}{s}\right)^{2-n} \exp\left(\frac{-s}{5r^2}\right) ds.$$

However, the function

$$x^{n-2} \exp\left(-\frac{x}{5}\right)$$

is bound from above, and the claim follows. The proof of (5.2) is exactly the same.

Applying our upper bound of the heat kernel for compact manifolds, we obtain the following eigenvalue estimates.

THEOREM 5.3. *Let M be a compact manifold with or without boundary. If $\partial M \neq \emptyset$, we assume that it is convex, i.e. $II \geq 0$. Suppose that the Ricci curvature of M is nonnegative. Let $\{0 = \mu_0 < \mu_1 \leq \mu_2 \leq ...\}$ be the set of eigenvalues of the Laplacian on M. When $\partial M \neq \emptyset$, we denote the set of Neumann eigenvalues also by $\{0 = \mu_0 < \mu_1 \leq \mu_2 \leq ...\}$ and the set of Dirichlet eigenvalues by $\{(0<)\lambda_1 < \lambda_2 \leq ...\}$. Then there exists a constant C_{13} depending only on n, such that*

$$\mu_k \geq \frac{C_{13}(k+1)^{2/n}}{d^2}$$

and

$$\lambda_k \geq \frac{C_{13} k^{2/n}}{d^2}$$

for all $k \geq 1$, where d is the diameter of M.

Proof. Let $H(x, y, t)$ be the appropriate heat kernel. Since the Dirichlet heat kernel is dominated from above by the Neumann heat kernel, for either boundary condition, by Theorem 3.2, we have the estimate

$$H(x, y, t) \leq C_{13} V^{-1}(B_x(\sqrt{t})).$$

Integrating both sides and applying (3.17), we have

$$\sum_{i=0}^{\infty} e^{-\mu_i t} \leq C_{13} \int_M V^{-1}(B_x(\sqrt{t})) \, dt \leq C_{13} \int_M f(t) \, dt, \tag{5.4}$$

where

$$f(t) = \begin{cases} \dfrac{V(0, d)}{V(0, \sqrt{t})} V^{-1}(B_x(d)), & \text{if } t \leq d \\ V^{-1}(B_x(d)), & \text{if } t \geq d. \end{cases}$$

Since $V(B_x(d)) = V(M)$, (5.4) yields

$$(k+1) e^{-\mu_k t} \leq C_{13} g(t), \tag{5.5}$$

where

$$g(t) = \begin{cases} \left(\dfrac{d}{\sqrt{t}}\right)^n, & \text{if } t \leq d \\ 1, & \text{if } t \geq d. \end{cases}$$

We multiply both sides by $e^{\mu_k t}$ and minimize the function $e^{\mu_k t} g(t)$ as follows:

Due to the fact that

$$\frac{d}{dt}(e^{\mu_k t} g(t)) = \mu_k e^{\mu_k t} g(t) + e^{\mu_k t} g'(t),$$

the function minimizes at t_0 must satisfy

$$\mu_k g(t_0) = -g'(t_0).$$

But $g'(t)=0$ when $t \geq d$, t_0 must be less than or equal to d. Hence

$$\mu_k \left(\frac{d}{\sqrt{t_0}} \right)^n = \frac{n}{2t_0} \left(\frac{d}{\sqrt{t_0}} \right)^n$$

and

$$t_0 = \frac{n}{2\mu_k}.$$

Substituting this value into (5.5) yields

$$k+1 \leq C_{13}(d\sqrt{\mu_k})^n.$$

A similar method gives estimates on λ_k also.

Remark. Obviously, using the same method as above, one can obtain eigenvalue estimates on compact manifolds with Ricci curvature bounded from below by $-K$, for some constant $K \geq 0$. In fact, the resulting lower bounds for the eigenvalues λ_k and μ_k depend only on n, K, d and k alone.

THEOREM 5.4. *Let M be a compact manifold with or without boundary. If $\partial M \neq \emptyset$, we assume that it is convex. Suppose the Ricci curvature of M is bounded from below by $-K$, for some constant $K \geq 0$, and also the sectional curvatures of M are bounded from above by $\varkappa > 0$. Let b_k be the kth Betti number for either the cohomology group $H^k(M)$ or the relative cohomology group $H^k(M, \partial M)$, then there exist constants C_{14} and C_{15} depending only on n such that*

$$b_1 \leq C_{14} \exp(C_{15} K d^2)$$

and

$$b_k \leq C_{14} \exp(C_{15}(K+\varkappa) d^2)$$

for $k > 1$, where d is the diameter of M.

Proof. To prove the estimate on b_1, we consider the harmonic representative of elements in $H^1(M)$ and $H^1(M, \partial M)$. The first is represented by harmonic 1-forms with absolute boundary condition, while the latter is represented by harmonic 1-forms with relative boundary condition. However, it was proved in [9] that the heat kernel $H_1(x, y, t)$ for 1-forms, with either boundary condition, can be dominated by

$$|H_1(x, x, t)| \leq n e^{kt} H(x, x, t).$$

Integrating both sides and applying our estimate for $H(x, x, t)$, yields

$$b_1 \leq C_{14} \int_M V^{-1}(B_x(\sqrt{t})) \exp(C_{15} Kt).$$

Setting $t = d^2$, the desired estimate follows.

To prove the estimates for $k \geq 2$, we follow the same procedure as above for the heat kernel for k-forms. In [9], it was proved that $\int_M |H_k(x, x, t)|$ can be estimated by

$$\int_M |H_k(x, x, t)| \leq \binom{n}{k} e^{Bt} \int_M H(x, x, t),$$

where B is a lower bound of the curvature term which arises in the Bochner formula. However, it is known that [12] B can be estimated by K and $\varkappa$. Hence the estimates are established.

§6. The Schrödinger operator

In this section, we will study the fundamental solution $H_\lambda(x, y, t)$ of the opertor

$$\Delta - \lambda^2 q - \frac{\partial}{\partial t}$$

where $q(x)$ is a fixed potential on M and $\lambda > 0$ is a parameter which is varying.

The behavior of $H_\lambda(x, y, t)$ as $\lambda \to \infty$ will be studied. In the case when $M = \mathbf{R}^n$, it was proved in [22] in relation to semi-classical approximation of multiple wells. Theorem 6.1 gives an asymptotic behavior of $H_\lambda(x, y, t)$ on arbitrary complete manifolds which enables one to push the argument in [22] through to the setting of a general manifold.

THEOREM 6.1. *Let M be a complete manifold without boundary. Suppose q is a C^2 function defined on M. For any $\lambda > 0$, we consider $H_\lambda(x, y, t)$, which is the fundamental solution of the equation*

$$\left(\Delta - \lambda^2 q - \frac{\partial}{\partial t}\right) u(x, t) = 0$$

on $M \times (0, \infty)$. Then

$$\lim_{\lambda \to \infty} \frac{\log H_\lambda(x, y, t/\lambda)}{\lambda} = -\varrho(x, y, t)$$

where $\varrho(x, y, t)$ is defined by (3.3).

Proof. For any given $x, y \in M$, let $B_p(R)$ be a geodesic ball with radius R containing x and y. Applying Theorem 2.1 to $H_\lambda(x, y, t)$, we have

$$H_\lambda(x, x, t_1) \leq H_\lambda(x, y, t_2) \left(\frac{t_2}{t_1}\right)^{n\alpha/2} \exp\left(A_\lambda(t_2 - t_1) + \varrho_{\alpha, R; \lambda}(x, y, t_2 - t_1)\right)$$

where

$$A_\lambda = C_7[\alpha R^{-1}\sqrt{K} + \alpha^3(\alpha-1)^{-1}R^{-2} + \lambda^{2/3}\gamma^{2/3}(\alpha-1)^{1/3}\alpha^{-1/3} + (\alpha\theta)^{1/2}\lambda + \alpha(\alpha-1)^{-1}K]$$

with K, θ, and γ as defined in Theorem 2.1. Also $\varrho_{\alpha, R; \lambda}(x, y, t)$ is the metric defined by (3.1) with $\lambda^2 q$ replacing q. Taking log of both sides, we have

$$\frac{\log H_\lambda(x, x, t_1/\lambda)}{\lambda} \leq \frac{\log H_\lambda(x, y, t_2/\lambda)}{\lambda} + \frac{n\alpha}{2\lambda}\log\frac{t_2}{t} + \frac{A_\lambda(t_2 - t_1)}{\lambda^2} + \frac{\varrho_{\alpha, R; \lambda}(x, y, (t_2 - t_1)/\lambda)}{\lambda}.$$

Letting $\lambda \to \infty$, and observing that

$$\frac{\varrho_{\alpha, R; \lambda}(x, y, t/\lambda)}{\lambda} = \varrho_{\alpha, R}(x, y, t)$$

and

$$\lim_{\lambda \to \infty} \frac{A_\lambda}{\lambda} = 0,$$

we conclude that

$$\lim_{\lambda \to \infty} \frac{\log H_\lambda(x, y, t_2/\lambda)}{\lambda} \geq \lim_{\lambda \to \infty} \frac{\log H_\lambda(x, x, t_1/\lambda)}{\lambda} - \varrho_{\alpha, R}(x, y, t_2 - t_1). \tag{6.1}$$

Letting $R \to \infty$, and $\alpha \to 1$, this gives

$$\lim_{\lambda \to \infty} \frac{\log H_\lambda(x, y, t_2/\lambda)}{\lambda} \geq \lim_{\lambda \to \infty} \frac{\log H_\lambda(x, x, t_1/\lambda)}{\lambda} - \varrho(x, y, t_2 - t_1). \tag{6.2}$$

We now claim that

$$\lim_{t_1 \to 0} \lim_{\lambda \to \infty} \frac{\log H_\lambda(x, x, t_1/\lambda)}{\lambda} \geq 0,$$

and the lower bound will follow. Indeed, if $q_0 \geq q$ on $B_p(2R)$, then the kernel $C^{-q_0 t}\tilde{H}(x, y, t)$ satisfies the equation

$$\left(\Delta - \lambda^2 q_0 - \frac{\partial}{\partial t}\right) e^{-\lambda^2 q_0 t} \tilde{H}(x, y, t) = 0,$$

with $\bar{H}(x, y, t)$ being the heat kernel with Dirichlet boundary condition on $B_p(2R)$. Hence, by the assumption $q_0 \geq q$ and the maximum principle,

$$H_\lambda(x, y, t) \geq e^{-\lambda^2 q_0 t} \bar{H}(x, y, t)$$

on $B_p(2R) \times B_p(2R) \times [0, \infty)$. In particular

$$\frac{\log H_\lambda(x, x, t_1/\lambda)}{\lambda} \geq -q_0 t_1 + \frac{\log \bar{H}(x, x, t_1/\lambda)}{\lambda}. \tag{6.3}$$

However, by the asymptotic formula for $\bar{H}(x, x, t)$ as $t \to 0$,

$$\lim_{\lambda \to \infty} \frac{\log \bar{H}(x, x, t_1/\lambda)}{\lambda} = \lim_{\lambda \to \infty} \frac{1}{t_1} \left(\frac{\log H(x, x, t_1/\lambda)}{t_1/\lambda} \right) = 0.$$

Hence, after letting $\lambda \to \infty$, (6.3) becomes

$$\lim_{\lambda \to \infty} \frac{\log H_\lambda(x, x, t_1/\lambda)}{\lambda} \geq -q_0 t_1,$$

and the claim follows by letting $t_1 \to 0$.

To establish the upper bound, we employ Theorem 3.3, which gives

$$\frac{\log H_\lambda(x, y, t/\lambda)}{\lambda} \leq \lambda^{-1} \log (1+\delta)^n V^{-1/2}(S_1) V^{-1/2}(S_2) + \lambda^{-2} A_\lambda \delta(2+\delta) t$$

$$+ \bar{\varrho}_{\alpha, R}(x, S_2, \delta(1+\delta) t) + \bar{\varrho}_{\alpha, R}(y, S_1, \delta t) \tag{6.4}$$

$$+ \bar{\varrho}(x, S_2, \delta(1+\delta) t) - \underline{\varrho}(x, S_1, (1+2\delta)(1+\delta) t).$$

Letting $\lambda \to \infty$, then $\alpha \to 1$ and $R \to \infty$, we get

$$\lim_{\lambda \to \infty} \frac{\log H_\lambda(x, y, t/\lambda)}{\lambda} \leq 2\bar{\varrho}(x, S_2, \delta(1+\delta) t) + \bar{\varrho}(y, S_1, \delta t) - \underline{\varrho}(x, S_1, (1+2\delta)(1+\delta) t).$$

Setting $S_2 = \{x\}$ and $S_1 = \{y\}$, we derive the inequality

$$\lim_{\lambda \to \infty} \frac{\log H_\lambda(x, y, t/\lambda)}{\lambda} \leq 2\varrho(x, x, \delta(1+\delta) t) + \varrho(y, y, \delta t) - \varrho(x, y, (1+2\delta)(1+\delta) t). \tag{6.5}$$

On the other hand, taking $\gamma: [0, 1] \to M$ to be the trivial curve with $\gamma(s) = x$, we see that

$$\varrho(x, x, t) \leq t q(x).$$

Hence, by letting $\delta \to 0$ in (6.5), the upper bound follows.

Remark. Since the techniques used in the above theorem are completely local in nature, Theorem 6.1 is still valid when the manifold is compact with or without boundary, for any boundary condition. In the case when $\partial M \neq \emptyset$, we need a version of the Harnack inequality which is valid for any points which are ε distance away from ∂M. Such a Harnack inequality can be derived using the method employed in § 1 and § 2. In that case, the estimate will depend on ε and the geometry of ∂M.

Appendix

We will establish the fact that the function $\varrho(x, y, t)$ defined in § 2 is Lipschitz for a locally bounded potential function q. Let r be the geodesic distance between y and z in M and γ_2 be a geodesic joining y to z which realizes distance. For any $\varepsilon > 0$, we can find a curve γ_1 parametrized by $s \in [0, 1]$ joining x to y such that

$$\varrho(x, y, t) + \varepsilon \geqslant \frac{1}{4t} \int_0^1 |\dot{\gamma}_1| \, ds + t \int_0^1 q(\gamma_1) \, ds.$$

We define a new curve γ by

$$\gamma(s) = \begin{cases} \gamma_1 \left(\dfrac{s}{1-r} \right), & \text{if } 0 \leqslant s \leqslant 1-r \\ \gamma_2(s+r-1), & \text{if } 1-r \leqslant s \leqslant 1. \end{cases}$$

Clearly $\gamma(s)$ is a curve joining x to z. Hence

$$\varrho(x, z, t) \leqslant \frac{1}{4t} \int_0^1 |\dot{\gamma}|^2 \, ds + t \int_0^1 q(\gamma(s)) \, ds$$

$$\leqslant \frac{1}{4t} \int_0^{1-r} |\dot{\gamma}_1|^2 (1-r)^{-2} \, ds + \frac{1}{4t} \int_{1-r}^1 |\dot{\gamma}_2|^2 \, ds + t \int_0^{1-r} q(\gamma_1(s)) \, ds + trq_0,$$

where q_0 is the supremum of $|q|$ in a neighborhood containing the curve γ. By a change of variable, the above inequality yields

$$\varrho(x, z, t) \leqslant \frac{1}{4t(1-r)} \int_0^1 |\dot{\gamma}_1|^2 \, ds + \frac{r}{4t} + t(1-r) \int_0^1 q(\gamma_1(s)) \, ds + trq_0$$

$$= \frac{1}{1-r} (\varrho(x, y, t) + \varepsilon) + \left(1 - r - \frac{1}{1-r} \right) t \int_0^1 q(\gamma_1(s)) \, ds + \frac{r}{4t} + trq_0.$$

Hence

$$\varrho(x, z, t) - \varrho(x, y, t) \leqslant \frac{r}{1-r} \varrho(x, y, t) + \frac{\varepsilon}{1-r} - \frac{r}{1-r} tq_0 + \frac{r}{4t}.$$

Letting $\varepsilon \to 0$, and using

$$\varrho(x, y, t) \leqslant \frac{r^2(x, y)}{4t} + t q_0,$$

we conclude that if $r(y, z) \leqslant \frac{1}{2}$ then

$$\varrho(x, z, t) - \varrho(x, y, t) \leqslant r(y, z) \cdot C,$$

where the constant C depends on q_0, t, and $r(x, y)$. Reversing the role of y and z yields the desired Lipschitz property of $\varrho(x, y, t)$.

References

[1] ARONSON, D. G., Uniqueness of positive weak solutions of second order parabolic equations. *Ann. Polon. Math.*, 16 (1965), 285–303.

[2] AZENCOTT, R., Behavior of diffusion semi-groups at infinity. *Bull. Soc. Math. France*, 102 (1974), 193–240.

[3] CHEEGER, J. & EBIN, D., *Comparison theorems in Riemannian geometry*. North-Holland Math. Library (1975).

[4] CHEEGER, J. & GROMOLL, D., The splitting theorem for manifolds of nonnegative Ricci curvature. *J. Differential Geom.*, 6 (1971), 119–128.

[5] CHEEGER, J., GROMOV, M. & TAYLOR, M., Finite propagation speed, kernel estimates for functions of the Laplace operator, and the geometry of complete Riemannian manifolds. *J. Differential Geom.*, 17 (1983), 15–33.

[6] CHEEGER, J. & YAU, S. T., A lower bound for the heat kernel. *Comm. Pure Appl. Math.*, 34 (1981), 465–480.

[7] CHENG, S. Y., LI, P. & YAU, S. T., On the upper estimate of the heat kernel of a complete Riemannian manifold. *Amer. J. Math.*, 103 (1981), 1021–1063.

[8] CHENG, S. Y. & YAU, S. T., Differential equations on Riemannian manifolds and their geometric applications. *Comm. Pure Appl. Math.*, 28 (1975), 333–354.

[9] DONNELLY, H. & LI, P., Lower bounds for the eigenvalues of Riemannian manifolds. *Michigan Math. J.*, 29 (1982), 149–161.

[10] FISCHER-COLBRIE, D. & SCHOEN, R., The structure of complete stable minimal surfaces in 3-manifolds of non-negative scalar curvature. *Comm. Pure Appl. Math.*, 33 (1980), 199–211.

[11] FRIEDMAN, A., On the uniqueness of the Cauchy problem for parabolic equations. *Amer. J. Math.*, 81 (1959), 503–511.

[12] GALLOT, S. & MEYER, D., Opérateur de courbure et Laplacien des formes différentielles d'une variété Riemannienne. *J. Math. Pures Appl.*, 54 (1975), 259–284.

[13] GROMOV, M., Paul Levy's isoperimetric inequality. IHES preprint.

[14] — Curvature, diameter, and Betti numbers. *Comment Math. Helv.*, 56 (1981), 179–197.

[15] KARP, L., & LI, P., The heat equation on complete Riemannian manifolds. Preprint.

[16] LI, P. & YAU, S. T., Estimates of eigenvalues of a compact Riemannian manifold. *Proc. Sympos. Pure Math.*, 36 (1980), 205–239.

[17] MAUREY, B. & MEYER, D., Un lemma de géométrie Hilbertienne et des applications à la géométrie Riemannienne. Preprint.

[18] MEYER, D., Un lemme de géométrie Hilbertienne et des applications à la géométrie Riemannienne. *C.R. Acad. Sci. Paris*, 295 (1982), 467–469.

[19] — Sur les hypersurfaces minimales des variétés Riemanniennes a courbure de Ricci positive ou nulle. *Bull. Soc. Math. France*, 111 (1983), 359–366.

[20] MOSER, J., A Harnack inequality for parabolic equations. *Comm. Pure Appl. Math.*, 17 (1964), 101–134.

[21] SERRIN, J. B., A uniqueness theorem for the parabolic equation $u_t = a(x) u_{xx} + b(x) u_x + c(x) u$. *Bull. Amer. Math. Soc.*, 60 (1954), 344.

[22] SIMON, B., Instantons, double wells and large deviations. *Bull. Amer. Math. Soc.*, 8 (1983), 323–326.

[23] VAROPOULOS, N., The Poisson kernel on positively curved manifolds. *J. Funct. Anal.*, 44 (1981), 359–380.

[24] — Green's functions on positively curved manifolds. *J. Funct. Anal.*, 45 (1982), 109–118.

[25] WIDDER, D. V., Positive temperature on the infinite rod. *Trans. Amer. Math. Soc.*, 55 (1944), 85–95.

[26] YAU, S. T., Harmonic functions on complete Riemannian manifolds. *Comm. Pure Appl. Math.*, 28 (1975), 201–228.

[27] — Some function-theoretic properties of complete Riemannian manifolds and their applications to geometry. *Indiana Univ. Math. J.*, 25 (1976), 659–670.