GLOBAL HEAT KERNEL ESTIMATES

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In this paper, by first deriving a global version of gradient estimates, we obtain both upper and lower bound estimates for the heat kernel satisfying Neumann boundary conditions on a compact Riemannian manifold with nonconvex boundary.

1. Introduction.

Let M be a compact Riemannian manifold with boundary ∂M . In their fundamental work [L-Y], P. Li and S.T. Yau had derived a version of gradient estimates for the positive solutions to the heat equations on M. Using those estimates, they then deduced a Harnack type inequality and demonstrated how that be applied to establish various upper and lower heat kernel bounds away from the boundary for both the Dirichlet and Neumann boundary conditions. Due to the interior nature of their gradient estimates, in general the heat kernel bounds do not extend up to the boundary. However, when the boundary is convex or the manifold is closed, the gradient estimates are valid globally, and so are the corresponding heat kernel bounds. In fact, in this case the upper and lower heat kernel bounds they obtained are sharp when the Ricci curvature of the manifold is nonnegative. One of our purposes in this paper is to demonstrate that a global version of their gradient estimates is also available when the boundary of M is nonconvex. This enables us to prove a global Harnack type inequality, with which one conveniently obtains an upper bound estimate valid up to the boundary for the heat kernel of M satisfying Neumann boundary conditions. As an application, we show that it together with a result of Varopoulos [V] readily gives us an estimate of the Neumann Sobolev constant of a general compact manifold with nonconvex boundary. Turning around, we then derive a lower bound estimate for the heat kernel. Notice that Croke [Cr] has estimated the isoperimetric constants for the closed manifolds in terms of various geometric data. The approach taken here does not allow us to estimate the isoperimetric constants.

The method employed here to estalish the gradient estimate essentially follows from [L-Y]. However, we shall point out that there are some technical

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complications due to the nonconvexity of the boundary as the estimates then necessarily involve the second fundamental form of ∂M and a so-called "interior rolling ball condition" for the boundary ∂M . The interior rolling ball condition was used by R. Chen in [C] to give an estimate of the first nonzero Neumann eigenvalue of M. We would also like to point out that the argument here can be easily adapted to more general cases, for example, the Schrödinger operators as considered in [L-Y]. But here we confine ourselves only to consider the heat operators.

Another problem that we want to consider in this paper is to establish the equivalence between the validity of a version of parabolic Harnack inequality and the existence of comparable upper and lower Gaussian bounds on the minimal heat kernel on a general complete manifold. It had been proved independently by Grigor'yan $[\mathbf{G}]$ and Saloff-Coste $[\mathbf{SC}]$ that a type of parabolic Harnack inequality is characterized by the volume doubling property and the weak-Neumann Poincaré inequality. On the other hand, it is not difficult to see from the argument in [L-Y] that the validity of such a parabolic Harnack inequality implies a Gaussian upper bound for the minimal heat kernel. Here, we first notice that such a Gaussian upper bound together with the parabolic Harnack inequality actually implies that there exists a comparable lower bound for the heat kernel. Then, with the help of a result by Fabes and Stroock [F-S] and the above mentioned characterization of the parabolic Harnack inequality, we show that the existence of such upper and lower bounds on the heat kernel actually implies that the parabolic Harnack inequality holds. As a consequence, one sees that the existence of such comparable upper and lower Gaussian bounds for the heat kernel is an invariant property under quasi-isometries on the manifold.

The paper is organized as follows. In Section 2, we derive the global gradient estimates for the positive solutions to the heat equation on a compact manifold with boundary and satisfying the Neumann boundary conditions. In Section 3, using the result from Section 2, we establish an upper bound for the heat kernel of a compact manifold which satisfies Neumann boundary conditions and as an application give an estimate of the Neumann Sobolev constant. Finally, in Section 4, we prove the equivalence between the validity of a type of parabolic Harnack inequality and the existence of Gaussian bounds on the heat kernel on a general complete manifold.

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2. Global Gradient Estimates.

Let (M^n, g) be an *n*-dimensional compact Riemannian manifold with boundary ∂M . Let $\frac{\partial}{\partial \nu}$ be the outward pointing unit normal vector to ∂M , and denote the second fundamental form of ∂M with respect to $\frac{\partial}{\partial \nu}$ by II. Our goal in this section is to derive estimates on the derivatives of positive solutions u(x,t) on $M \times (0,\infty)$ of the equation

(2.1)
$$\begin{cases} (\Delta - \frac{\partial}{\partial t})u(x,t) = 0\\ \frac{\partial u}{\partial \nu} \mid_{\partial M} = 0. \end{cases}$$

Our estimates are of global nature and will be valid up to the boundary of M. The corresponding interior estimates were previously established by P. Li and S.T. Yau in their fundamental work [L-Y]. In fact, we shall use the same method developed by them in [L-Y].

Definition 2.1. ∂M is said to satisfy the "interior rolling R-ball" condition if for each point $p \in \partial M$ there is a geodesic ball $B_q(\frac{R}{2})$, centered at $q \in M$ with radius $\frac{R}{2}$, such that $p = B_q(\frac{R}{2}) \cap \partial M$ and $B_q(\frac{R}{2}) \subset M$.

Theorem 2.2. Let (M^n, g) be a compact Riemannian manifold with boundary ∂M . Suppose that ∂M satisfies the "interior rolling R-ball" condition. Let K and H be nonnegative constants such that the Ricci curvature Ric_M of M is bounded below by -K and the second fundamental form II of ∂M is bounded below by -H. By choosing R small, we have for any positive solution u(x,t) of (2.1) on $M \times (0,\infty)$,

(2.2)
$$\frac{|\nabla u|^2}{u^2} - \alpha \frac{u_t}{u} \le C_1 + \frac{C_2}{t}$$

on $M \times (0, \infty)$ for all constant

$$\alpha > (H+1)^2$$
 and $0 < \beta < \frac{1}{2}$

where

$$C_{1} = \frac{6n\alpha(\alpha-1)(1+H)^{7}K}{(\alpha-(1+H)^{2})^{2}} + \frac{309n^{2}\alpha^{3}(\alpha-1)(1+H)^{10}H}{(\alpha-(1+H)^{2})^{4}R^{2}\beta}$$
$$C_{2} = \frac{n\alpha^{2}(\alpha-1)^{2}(1+H)^{4}}{(2-\beta)(1-\beta)(\alpha-(1+H)^{2})^{2}}.$$

Proof. Following [C], we define a function on M by $\phi(x) = \psi\left(\frac{r(x)}{R}\right)$, where r(x) denotes the distance from $x \in M$ to ∂M and $\psi(r)$ is a nonnegative

 C^2 -function defined on $[0,\infty)$ such that

$$\begin{cases} \psi(r) \le H \text{ if } r \in [0, 1/2) \\ \psi(r) = H \text{ if } r \in [1, \infty) \end{cases}$$

with $\psi(0) = 0$, $0 \leq \psi'(r) \leq 2H$, $\psi'(0) = H$ and $\psi''(r) \geq -H$. Let $f = \log u$. Then $(\Delta - \frac{\partial}{\partial t})f(x,t) = -|\nabla f|^2(x,t)$. Consider for every $\varepsilon > 0$

$$F(x,t) = t\left\{(1+\phi(x))^2(|\nabla f|^2(x,t)+\varepsilon) - \alpha f_t(x,t)\right\}.$$

For any fixed $T < \infty$, since F(x,t) is continuous on $\overline{M} \times [0,T]$, there exists $(p,t_0) \in \overline{M} \times [0,T]$ at which F achieves its maximum. We may assume that $F(p,t_0) > 0$ as otherwise (2.2) follows trivially.

Claim 1. $p \in \overline{M} \setminus \partial M$.

In fact, if $p \in \partial M$, then $\frac{\partial F}{\partial \nu}(p,t_0) \geq 0$. Let e_1, e_2, \ldots, e_n be an orthonormal frame at p with $e_n = \nu$. Notice that $f_n = f_{\nu} = \frac{\frac{\partial u}{\partial \nu}}{u} = 0$ on ∂M . Therefore, denoting $\varphi(x) = (1 + \phi(x))^2$, we have

$$0 \leq \frac{\partial F}{\partial \nu}(p, t_0) = t_0 \left(\frac{\partial \varphi}{\partial \nu} (|\nabla f|^2 + \varepsilon) + 2\varphi \sum_{i=1}^n f_i f_{i\nu} - \alpha f_{\nu t} \right) (p, t_0).$$

Since $f_{\nu} = 0$ on ∂M and $t_0 > 0$, we conclude that $\frac{\partial \varphi}{\partial \nu} \cdot \frac{1}{\varphi} + \frac{2\sum_{i=1}^{n-1} f_i f_{i\nu}}{|\nabla f|^2 + \varepsilon} \ge 0$ at (p, t_0) . By a direct computation, one shows that

$$\sum_{i=1}^{n-1} f_i f_{i\nu} = -\operatorname{II}(\nabla f, \nabla f) \le H |\nabla f|^2.$$

Thus at (p, t_0) , if we choose R < 1, then

$$\begin{split} & \frac{\partial \varphi}{\partial \nu} \frac{1}{\varphi} + \frac{2 \sum_{i=1}^{n-1} f_i f_{i\nu}}{|\nabla f|^2 + \varepsilon} \\ & \leq -\frac{2H}{R} + \frac{2H |\nabla f|^2}{|\nabla f|^2 + \varepsilon} < 0. \end{split}$$

This is a contradiction and the claim follows. Thus, F(x,t) achieves its maximum at $(p, t_0) \in (\overline{M} \setminus \partial M) \times (0, T]$.

Hence at (p, t_0) , $\nabla F = 0$, $\frac{\partial F}{\partial t} \ge 0$ and $\Delta F \le 0$. In the following, all the computations are performed at the point (p, t_0) and the summation convention is used with indices i and j both moving between 1 and n. Direct computation gives us

$$\Delta F = t \left(\Delta \varphi \cdot \left(|\nabla f|^2 + \varepsilon \right) + \varphi \Delta |\nabla f|^2 + 2\nabla \varphi \cdot \nabla |\nabla f|^2 - \alpha (\Delta f)_t \right)$$

= $t \left(\Delta \varphi \left(|\nabla f|^2 + \varepsilon \right) + 2\varphi (f_{ij}^2 + f_i f_{ijj}) + 2\nabla \varphi \cdot \nabla |\nabla f|^2 - \alpha (\Delta f)_t \right).$

Since

$$f_i f_{ijj} = f_i f_{jji} + \operatorname{Ric}(\nabla f, \nabla f)$$
$$\geq \nabla f \cdot \nabla(\Delta f) - K |\nabla f|^2$$

and $\Delta f = f_t - |\nabla f|^2$, we obtain

$$\begin{split} \Delta F &\geq t \Big\{ \Delta \varphi \left(|\nabla f|^2 + \varepsilon \right) + 2\varphi \left(f_{ij}^2 - K |\nabla f|^2 + \nabla f \cdot \nabla (\Delta f) \right) \\ &+ 2\nabla \varphi \cdot \nabla |\nabla f|^2 - \alpha \left(f_t - |\nabla f|^2 \right)_t \Big\}. \end{split}$$

Also
$$F_t = \varphi(|\nabla f|^2 + \varepsilon) - \alpha f_t + t(\varphi|\nabla f|_t^2 - \alpha f_{tt})$$
. Thus $0 \ge \Delta F - \frac{\partial F}{\partial t}$ implies
 $0 \ge t \Big\{ \Delta \varphi \left(|\nabla f|^2 + \varepsilon \right) + 2\varphi f_{ij}^2 - 2K\varphi |\nabla f|^2 + 2\varphi \nabla f \cdot \nabla \left(f_t - |\nabla f|^2 \right) + 2\nabla \varphi \cdot \nabla |\nabla f|^2 + (\alpha - \varphi) |\nabla f|_t^2 \Big\} - \varphi \left(|\nabla f|^2 + \varepsilon \right) + \alpha f_t$

$$= t \Big\{ \varepsilon \Delta \varphi + (\Delta \varphi - 2K\varphi) |\nabla f|^2 + 2\varphi f_{ij}^2 \Big\} - \frac{F}{t}$$

$$+ t \Big\{ 2\nabla \varphi \cdot \nabla |\nabla f|^2 - 2\varphi \nabla f \cdot \nabla |\nabla f|^2 + 2\alpha \nabla f \cdot \nabla f_t \Big\}.$$

Using the fact that

$$\nabla F = t \left\{ \left(|\nabla f|^2 + \varepsilon \right) \nabla \varphi + \varphi \nabla |\nabla f|^2 - \alpha \nabla f_t \right\} = 0,$$

we get

$$\begin{split} 0 &\geq t \left\{ \varepsilon \Delta \varphi + (\Delta \varphi - 2K\varphi) |\nabla f|^2 + 2\varphi f_{ij}^2 \right\} - \frac{F}{t} \\ &+ 2t \nabla \varphi \cdot \nabla |\nabla f|^2 + 2t \left(|\nabla f|^2 + \varepsilon \right) \nabla \varphi \cdot \nabla f \end{split}$$

$$\begin{split} &\geq t \left\{ \varepsilon \Delta \varphi + (\Delta \varphi - 2K\varphi) |\nabla f|^2 + 2\varphi f_{ij}^2 \right\} - \frac{F}{t} \\ &\quad + 4t \varphi_i f_j f_{ij} - 2t |\nabla \varphi| |\nabla f|^3 - 2t |\nabla \varphi| |\nabla f| \varepsilon \\ &\geq 2\varphi t f_{ij}^2 + t (\Delta \varphi - 2K\varphi) |\nabla f|^2 + \varepsilon t \Delta \varphi - \frac{F}{t} \\ &\quad - \frac{4t}{\beta} |\nabla \varphi|^2 |\nabla f|^2 - \beta t f_{ij}^2 - 2t |\nabla \varphi| |\nabla f|^3 - |\nabla \varphi|^2 t \varepsilon - |\nabla f|^2 t \varepsilon \\ &\geq (2\varphi - \beta) t f_{ij}^2 + t \left(\Delta \varphi - 2K\varphi - \frac{4}{\beta} |\nabla \varphi|^2 - \varepsilon \right) |\nabla f|^2 \\ &\quad - 2t |\nabla \varphi| |\nabla f|^3 + \varepsilon t \left(\Delta \varphi - |\nabla \varphi|^2 \right) - \frac{F}{t}. \end{split}$$

Since
$$\sum f_{ij}^2 \ge \sum f_{ii}^2 \ge \frac{(\sum f_{ii})^2}{n} = \frac{(\Delta f)^2}{n} = \frac{(|\nabla f|^2 - f_t)^2}{n},$$

(2.3) $0 \ge \frac{(2\varphi - \beta)t^2}{n} \left(|\nabla f|^2 - f_t\right)^2 - 2t^2 |\nabla \varphi| |\nabla f|^3 + t^2 \left(\Delta \varphi - 2K\varphi - \frac{4}{\beta} |\nabla \varphi|^2 - \varepsilon\right) |\nabla f|^2 + \varepsilon t^2 \left(\Delta \varphi - |\nabla \varphi|^2\right) - F.$

Claim 2.

$$(|\nabla f|^2 - f_t)^2 \ge \frac{(1-\beta)\left(\alpha - (1+H)^2\right)^2}{(\alpha - 1)^2(H+1)^4} \left(\varphi\left(|\nabla f|^2 + \varepsilon\right) - f_t\right)^2 - \frac{2\varepsilon^2}{\beta}.$$

In fact, using the elementary inequality $a^2 \ge (1-\beta)(a+b)^2 - \frac{2}{\beta}b^2$, we conclude that

$$\left(|\nabla f|^2 - f_t\right)^2 \ge (1 - \beta) \left(|\nabla f|^2 + \varepsilon - f_t\right)^2 - \frac{2\varepsilon^2}{\beta}.$$

On the other hand, $F\geq 0$ at $(p,t_0),$ hence

$$\varphi\left(|\nabla f|^2 + \varepsilon\right) - \alpha f_t \ge 0.$$

In other words,

(2.4)
$$f_t \le \frac{\varphi}{\alpha} \left(|\nabla f|^2 + \varepsilon \right).$$

Therefore

$$(1-\beta)\left(|\nabla f|^2 + \varepsilon - f_t\right)^2 - \frac{(1-\beta)\left(\alpha - (1+H)^2\right)^2}{(\alpha-1)^2(H+1)^4}\left(\varphi\left(|\nabla f|^2 + \varepsilon\right) - f_t\right)^2$$

$$\begin{split} &= (1-\beta) \left[\left(|\nabla f|^2 + \varepsilon - f_t \right) + \frac{\alpha - (1+H)^2}{(\alpha - 1)(H+1)^2} \left(\varphi \left(|\nabla f|^2 + \varepsilon \right) - f_t \right) \right] \\ &\quad \cdot \left[\left(|\nabla f|^2 + \varepsilon - f_t \right) - \frac{\alpha - (1+H)^2}{(\alpha - 1)(H+1)^2} \left(\varphi \left(|\nabla f|^2 + \varepsilon \right) - f_t \right) \right] \\ &= (1-\beta) \left[\left(1 + \varphi \frac{\alpha - (1+H)^2}{(\alpha - 1)(H+1)^2} \right) \left(|\nabla f|^2 + \varepsilon \right) \\ &\quad - \left(1 + \frac{\alpha - (1+H)^2}{(\alpha - 1)(H+1)^2} \right) f_t \right] \\ &\quad \cdot \left[\left(1 - \varphi \frac{\alpha - (1+H)^2}{(\alpha - 1)(H+1)^2} \right) \left(|\nabla f|^2 + \varepsilon \right) - \left(1 - \frac{\alpha - (1+H)^2}{(\alpha - 1)(H+1)^2} \right) f_t \right]. \end{split}$$

Using (2.4), one easily checks that the above expression is nonnegative and the claim is verified. Using the claim and (2.3), we obtain

$$(2.5) \quad 0 \geq \frac{(2\varphi - \beta)t^2}{n} \cdot \frac{(1 - \beta)(\alpha - (1 + H)^2)^2}{(\alpha - 1)^2(1 + H)^4} \left(\varphi \left(|\nabla f|^2 + \varepsilon\right) - f_t\right)^2 - 2t^2 |\nabla \varphi| |\nabla f|^3 + t^2 \left(\Delta \varphi - 2K\varphi - \frac{4}{\beta} |\nabla \varphi|^2 - \varepsilon\right) |\nabla f|^2 + \varepsilon t^2 \left(\Delta \varphi - |\nabla \varphi|^2 - \frac{2\varepsilon(2\varphi - \beta)}{n\beta}\right) - F.$$

Let $y = \varphi(|\nabla f|^2 + \varepsilon)$ and $z = f_t$. Then

$$(2.6) \quad (y-z)^2 = \left[\frac{1}{\alpha}(y-\alpha z) + \frac{\alpha-1}{\alpha}y\right]^2$$
$$= \frac{1}{\alpha^2}(y-\alpha z)^2 + \left(\frac{\alpha-1}{\alpha}\right)^2 y^2 + \frac{2(\alpha-1)}{\alpha^2}y(y-\alpha z)$$
$$\ge \frac{1}{\alpha^2 t^2}F^2 + \left(\frac{\alpha-1}{\alpha}\right)^2 y^2 \quad \text{as} \quad y-\alpha z = \frac{F}{t} > 0.$$

Combining (2.5) and (2.6), we get

$$(2.7) \quad 0 \geq \frac{(2\varphi - \beta)(1 - \beta)(\alpha - (1 + H)^2)^2}{n\alpha^2(\alpha - 1)^2(1 + H)^4}F^2 - F + \frac{(2\varphi - \beta)(1 - \beta)t^2(\alpha - (1 + H)^2)^2}{n\alpha^2(1 + H)^4}y^2 - 2t^2|\nabla\varphi||\nabla f|^3 + t^2\left(\Delta\varphi - 2K\varphi - \frac{4}{\beta}|\nabla\varphi|^2 - \varepsilon\right)|\nabla f|^2$$

$$+ \varepsilon t^2 \left(\Delta \varphi - |\nabla \varphi|^2 - \frac{2\varepsilon (2\varphi - \beta)}{n\beta} \right).$$

By $[\mathbf{C}]$, if we choose R sufficiently small, then

$$\Delta\phi \ge -\frac{2(n-1)H(2H+1)}{R} - \frac{H}{R^2}.$$

Therefore,

$$\begin{split} \Delta \varphi &= 2(1+\phi)\Delta \phi + 2|\nabla \phi|^2\\ &\geq 2(1+H)\left(-\frac{2(n-1)H(3H+1)}{R} - \frac{H}{R^2}\right)\\ &= -C_3. \end{split}$$

Hence

$$(2.8) \qquad \frac{(2\varphi - \beta)(1 - \beta)(\alpha - (1 + H)^2)^2}{n\alpha^2(1 + H)^4}y^2 - 2|\nabla\varphi||\nabla f|^3 \\ + \left(\Delta\varphi - 2K\varphi - \frac{4}{\beta}|\nabla\varphi|^2 - \varepsilon\right)|\nabla f|^2 \\ \ge \frac{(\alpha - (1 + H)^2)^2}{2n\alpha^2(1 + H)^4}y^2 - 8H(H + 1)y^{\frac{3}{2}} - \left(C_3 + 2K(1 + H)^2 + \frac{64}{\beta}H^2(H + 1)^2 + \varepsilon\right)y.$$

Consider $Ay^2 - By^{\frac{3}{2}} - Cy$, where A, B, C all are positive. Clearly

$$(2.9) \quad Ay^{2} - By^{\frac{3}{2}} - Cy = \frac{A}{2}y^{2} + \frac{A}{2}y^{2} - By^{\frac{3}{2}} + \frac{B^{2}}{2A}y - \left(C + \frac{B^{2}}{2A}\right)y$$
$$\geq \frac{A}{2}y^{2} - \left(C + \frac{B^{2}}{2A}\right)y = \frac{A}{2}y^{2} - \left(C + \frac{B^{2}}{2A}\right)y + D^{2} - D^{2}$$
$$\geq -D^{2}, \quad \text{where} \quad D^{2} = \frac{\left(C + \frac{B^{2}}{2A}\right)^{2}}{2A}.$$

Applying (2.9) to (2.8), we conclude from (2.7) that

(2.10)
$$0 \ge \frac{(2\varphi - \beta)(1 - \beta)(\alpha - (1 + H)^2)^2}{n\alpha^2(\alpha - 1)^2(1 + H)^4}F^2 - F$$

$$+ \varepsilon t^2 \left(\Delta \varphi - |\nabla \varphi|^2 - \frac{2\varepsilon(2\varphi - \beta)}{n\beta} \right) - D^2 t^2$$

where $D^2 = \frac{(C + \frac{B^2}{2A})^2}{2A}$, and $A = \frac{(\alpha - (1 + H)^2)^2}{2n\alpha^2(1 + H)^4}$, B = 8H(H + 1) and $C = (C_3 + 2K(1 + H)^2 + \frac{64}{\beta}H^2(H + 1)^2 + \varepsilon)$. From (2.10), one easily obtains

$$(2.11) F \le \frac{1 + \sqrt{1 + 4PQ}}{2P},$$

where

$$P = \frac{(2\varphi - \beta)(1 - \beta)(\alpha - (1 + H)^2)^2}{n\alpha^2(\alpha - 1)^2(1 + H)^4}$$

and

$$Q = D^{2}t^{2} - \varepsilon t^{2} \left(\Delta \varphi - |\nabla \varphi|^{2} - \frac{2\varepsilon(2\varphi - \beta)}{n\beta} \right)$$

But

$$|\nabla f|^2 - \alpha f_t \le \varphi \left(|\nabla f|^2 + \varepsilon \right) - \alpha f_t = \frac{F}{t}.$$

Thus by (2.11) and letting $\varepsilon \to 0$, we have

$$\begin{split} |\nabla f|^2 - \alpha f_t &\leq n\alpha^2 (\alpha - 1)^2 (1 + H)^4 \\ & \cdot \frac{1 + \sqrt{1 + 8D^2 t^2 \left(\alpha - (1 + H)^2\right)^2 / n\alpha^2 (\alpha - 1)^2 (1 + H)^2}}{2(2\varphi - \beta)(1 - \beta) \left(\alpha - (1 + H)^2\right)^2 t} \\ &\leq \frac{n\alpha^2 (\alpha - 1)^2 (1 + H)^4 \left(1 + 1 + \frac{3Dt(\alpha - (1 + H)^2)}{\sqrt{n\alpha} (\alpha - 1)(1 + H)}\right)}{2(2\varphi - \beta)(1 - \beta) \left(\alpha - (1 + H)^2\right)^2 t}. \end{split}$$

In conclusion,

$$\frac{\nabla u|^2}{u^2} - \alpha \frac{u_t}{u} \le C_1 + \frac{C_2}{t}$$

where

$$C_1 \le \frac{6n\alpha(\alpha-1)(1+H)^7 K}{\left(\alpha - (1+H^2)^2\right)^2} + \frac{309n^2\alpha^3(\alpha-1)(1+H)^{10}H}{\left(\alpha - (1+H)^2\right)^4 R^2\beta}$$

and

$$C_2 \le \frac{n\alpha^2(\alpha-1)^2(1+H)^4}{(2\varphi-\beta)(1-\beta)(\alpha-(1+H)^2)^2} \le \frac{n\alpha^2(\alpha-1)^2(1+H)^4}{(2-\beta)(1-\beta)(\alpha-(1+H)^2)^2}.$$

The proof is completed.

Corollary 2.3 ([L-Y]). Let M and u be as in Theorem 2.2. If the boundary ∂M of M is convex, i.e., H = 0, then for any $\alpha > 1$,

$$\frac{|\nabla u|^2}{u^2} - \alpha \frac{u_t}{u} \le C_3 + \frac{C_4}{t},$$

where $C_3 = \frac{6n\alpha K}{\alpha - 1}$ and $C_4 = \frac{n\alpha^2}{2}$. If furthermore the Ricci curvature of M is also nonnegative, then

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

Proof. In the first case that H = 0, we use Theorem 2.2 and let β approach to 0. For the second case, since K = 0, one can also let α approach to 1.

Remark. In our estimate, R is chosen to be a positive constant less than 1 and is dependent on the upper bound of the sectional curvature of the manifold near the boundary. The upper bound of R is explicitly determined by

$$\sqrt{K_R} \tan\left(R\sqrt{K_R}\right) \le \frac{H}{2} + \frac{1}{2}$$

and

$$\frac{H}{\sqrt{K_R}}\tan\left(R\sqrt{K_R}\right) \le \frac{1}{2}$$

where K_R is the upper bound of the sectional curvature on the set $M_R = \{x \in M \mid r(x) \leq R\}$ (see [C]).

3. Estimate of Sobolev Constants.

In this section, we shall utilize the global gradient estimate in the previous section to derive an upper bound for the heat kernel satisfying Neumann boundary conditions on a general compact manifold with nonconvex boundary. The result is then used to estimate the Neumann Sobolev constants. Previously, Croke [Cr] has obtained the estimates of Neumann isoperimetric constants for the manifolds without boundary. Our approach here does not allow us to estimate the isoperimetric constants. Thus, it is still left open to give an estimate of the isoperimetric constants for a compact manifold with nonconvex boundary.

First, we establish the following Harnack inequality.

Theorem 3.1. Let M be a compact manifold with boundary ∂M . Suppose that the Ricci curvature of M satisfies $\operatorname{Ric}_M \geq -K$, $K \geq 0$ and the second fundamental form of ∂M with respect to outward pointing normal ν satisfies $II \geq -H$, $H \geq 0$. Suppose that ∂M also satisfies the "interior rolling Rball condition" with R chosen small (see the remark at the end of Section 2). Then for any positive function u(x, t) on $M \times (0, \infty)$ satisfying

$$\begin{cases} (\Delta - \frac{\partial}{\partial t})u = 0\\ \frac{\partial u}{\partial \nu} \mid_{\partial M} = 0, \end{cases}$$

 $\begin{array}{ll} u(x_1,t_1) &\leq \ u(x_2,t_2) \left(\frac{t_2}{t_1}\right)^{C_5} \exp\left(\frac{\alpha r^2(x_1,x_2)}{4(t_2-t_1)} + C_6(t_2-t_1)\right) \ for \ any \ \alpha \\ (1+H)^2 \ and \ 0 < \beta < \frac{1}{2}, \ x_1, x_2 \in M \ and \ 0 < t_1 < t_2 < \infty, \ where \end{array}$

$$C_5 = \frac{n\alpha(\alpha - 1)^2(1 + H)^4}{(2 - \beta)(1 - \beta)(\alpha - (1 + H)^2)^2},$$

$$C_6 = \frac{6n(\alpha - 1)(1 + H)^7K}{(\alpha - (1 + H)^2)^2} + \frac{309n^2\alpha^2(\alpha - 1)(1 + H)^{10}H}{(\alpha - (1 + H)^2)^4 R^2\beta}$$

Proof. The proof uses (2.2) and proceeds as Theorem 2.1 in $[\mathbf{L}-\mathbf{Y}]$. Hence it is omitted here.

Applying Theorem 3.1 and arguing as in $[\mathbf{L}-\mathbf{Y}]$, one conveniently obtains an estimate of heat kernel of M satisfying Neumann boundary condition.

Theorem 3.2. Let M be as in Theorem 3.1. Let H(x, y, t) be the heat kernel of M satisfying Neumann boundary conditions. Then for any $\alpha > (1+H)^2$, $0 < \beta < \frac{1}{2}$ and $\delta > 0$, and x, y on M,

$$\begin{split} H(x,y,t) \\ &\leq (1+\delta)^{2C_5} \exp\left(\frac{1+\alpha}{\delta}\right) V_x^{-\frac{1}{2}} \left(\sqrt{t}\right) V_y^{-\frac{1}{2}} \left(\sqrt{t}\right) \exp\left(-\frac{r^2(x,y)}{(4+\delta)t} + C_6 \delta t\right), \end{split}$$

where C_5 and C_6 are given in Theorem 3.1.

In order to improve the above estimate for t large, we use a method due to S.Y. Cheng and P. Li [C-L].

Lemma 3.3 ([C-L]). Let $l_1(M)$ be the first nonzero eigenvalue of M satisfying Neumann boundary condition, then for any fixed t_0 and all $t \ge t_0$,

$$H(x, x, t) \le \frac{1}{V(M)} + H(x, x, t_0) \exp(-l_1(M)(t - t_0)).$$

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Proof. Let $\bar{H}(x, y, t) = H(x, y, t) - \frac{1}{V(M)}$. Then $\int_M \bar{H}(x, y, t) dy = 0$. But by the semigroup property of H(x, y, t), we have

$$\begin{split} \frac{\partial}{\partial t}\bar{H}(x,x,t) &= \frac{\partial}{\partial t}\int_{M}\bar{H}^{2}\left(x,y,\frac{t}{2}\right)dy\\ &= \int_{M}\bar{H}\left(x,y,\frac{t}{2}\right)\Delta\bar{H}\left(x,y,\frac{t}{2}\right)dy\\ &= -\int_{M}|\nabla\bar{H}|^{2}\left(x,y,\frac{t}{2}\right)dy\\ &\leq -l_{1}(M)\int_{M}\bar{H}^{2}\left(x,y,\frac{t}{2}\right)dy\\ &= -l_{1}(M)\bar{H}(x,x,t). \end{split}$$

Integrating this differential inequality from t_0 to t gives

$$\bar{H}(x, x, t) \leq \bar{H}(x, x, t_0) \exp(-l_1(M)(t - t_0)).$$

Now the lemma follows using the definition of $\overline{H}(x, y, t)$.

If we choose $t_0 = d^2$, where d is the diameter of M, then by Lemma 3.3 and Theorem 3.2 together with the estimate of $l_1(M)$ obtained by R. Chen in [C], we obtain the following estimate for the heat kernel of M satisfying Neumann boundary conditions.

Theorem 3.4. Let M be as in Theorem 3.1. Then for t > 0 and x, y in M,

$$H(x, y, t) \le \frac{1}{V(M)} + C_7 V_x^{-\frac{1}{2}} \left(\sqrt{t}\right) V_y^{-\frac{1}{2}} \left(\sqrt{t}\right) \exp\left(-\frac{r^2(x, y)}{5t} - C_8 t\right),$$

where C_7 and C_8 are two positive constants which only depend on d, K, H, R and n and can be explicitly computed.

Finally, we want to use the above heat kernel bound to estimate the Neumann Sobolev constant of M. Consider the following type of Sobolev inequality

$$\inf_{k \in \mathbf{R}} \left(\int_M |f - k|^{\frac{2n}{n-2}} \right)^{\frac{n-2}{n}} \le C(S) \int_M |\nabla f|^2 \quad \text{for all } f \in C^\infty(\bar{M}).$$

The minimum constant C(S) is called the Neumann Sobolev constant of M. Using a result of Varopoulos $[\mathbf{V}]$, we can now estimate C(S) from above in terms of geometric data of M. But before we do that, we need the following lemma.

Lemma 3.5. Let M be as in Theorem 3.1. Then $V_x(t) \ge C(d, K, H, V, R)t^n$ for some constant C(d, K, H, V, R) > 0 and all $x \in M$ and $t \le R$, where V = V(M).

Proof. We first note that M satisfies volume doubling property by Theorem 3.1 and 3.4 (see [SC]).

Claim. For each $x \in M$ and $t \leq R$, there exists a geodesic ball $B_p(\frac{t}{6}) \subset B_x(t)$ such that $B_p(\frac{t}{6})$ does not intersect ∂M .

In fact, the claim is trivially true if the distance $d(x, \partial M) = r(x) \geq \frac{t}{2}$. Thus we consider the case $r(x) < \frac{t}{2} \leq \frac{R}{2}$. Let $y \in \partial M$ be such that r(x, y) = r(x). Clearly, we have $B_y(\frac{t}{2}) \subset B_x(t)$. On the other hand, by the interior rolling R-ball condition, there exists a ball $B_q(\frac{R}{2})$ such that it only intersects ∂M at y. Now let γ be a minimal geodesic connecting y and q. Choose a point p on γ such that $r(p, y) = \frac{t}{4}$. Then it is easy to check that $B_p(\frac{t}{6}) \subset B_y(\frac{t}{2}) \subset B_x(t)$. Also, $B_p(\frac{t}{6}) \subset B_q(\frac{R}{2})$. Since $r(p, y) > \frac{t}{6}$, y is not in $B_p(\frac{t}{6})$. Therefore $B_p(\frac{t}{6})$ does not intersect ∂M and the claim follows.

Now we divide the proof of the lemma into two cases.

Case (i): $r(x) < \frac{R}{2}$.

Let $M_R = \{x \in M : r(x) \leq R\}$. Then $B_x(\frac{t}{2}) \subset M_R$. By the claim, there exists $B_p(\frac{t}{12}) \subset B_x(\frac{t}{2})$ and $B_p(\frac{t}{12})$ has no intersection with ∂M . Since by the choice of R, $\sqrt{K_R} \tan(R\sqrt{K_R}) \leq \frac{H+1}{2}$, where K_R is an upper bound of the sectional curvature on M_R . Therefore $K_R \leq \frac{H+1}{2R}$. So the injectivity radius of the set M_R can be estimated from below by a constant C(V, R, H, d). In particular, we conclude that $V_p(\frac{t}{12}) \geq C(V, R, H, d)t^n$ for some constant C(V, R, H, d) > 0. Thus we proved the lemma for this case.

Case (ii): $r(x) \ge \frac{R}{2}$.

In this case, we first show $V_x(r(x)) \geq C(V, R, H, d)$. In fact, arguing as in the claim, we conclude that there exists a ball $B_p(\frac{R}{12}) \subset M_{\frac{R}{3}}$ such that $B_p(\frac{R}{12}) \subset B_x(r(x))$. From case (i), we obtain $V_x(r(x)) \geq C(V, R, H, d)$. Now inside the ball $B_x(r(x))$ we may apply the Bishop volume comparison theorem. Notice that $r(x) \leq d$. We conclude that for $t \leq \frac{R}{2}$,

$$\frac{V_x(r(x))}{V_x(t)} \le \frac{V_K(r(x))}{V_K(t)} \le \frac{V_K(d)}{V_K(t)},$$

where $V_K(r)$ denotes the volume of the geodesic ball of radius r in the space form of constant curvature $\frac{-K}{n-1}$. Putting together the preceding facts, we see that $V_x(t) \ge C(d, V, K, H, R)t^n$. The lemma is proved.

Combining Theorem 3.4 and Lemma 3.5, we obtain the following corollary.

Corollary 3.6. Let M be as in Theorem 3.1. Then for all t > 0 and $x \in M$,

(3.12)
$$H(x, x, t) \le \frac{1}{V(M)} + At^{-\frac{n}{2}}$$

where $n = \dim M$ and A = A(d, H, R, K, V) a positive constant which can be computed explicitly.

The following theorem is a consequence of a result in $[\mathbf{V}]$ and the preceding corollary.

Theorem 3.7. Let M be as in Theorem 3.1. Then the Neumann Sobolev constant C(S) of M satisfies

$$C(S) \le C(n)A^{\frac{2}{n}},$$

where C(n) is a constant only depending on n and A is the constant in (3.12). In particular, $C(S) \leq C(d, H, R, K, V)$ a constant which can be explicitly computed.

Using Theorem 3.7, we now derive a lower bound estimate for the heat kernel H(x, y, t). The following proof is adapted from [C-L].

Theorem 3.8. Let M be as in Theorem 3.1. Then the heat kernel H(x, y, t) of M satisfying the Neumann boundary conditions has estimates

$$\frac{1}{V(M)} - C_9 t^{-n/2} \le H(x, y, t) \le \frac{1}{V(M)} + C_{10} t^{-n/2},$$

where C_9 and C_{10} are two positive constants depending on d, K, H, R and V.

Proof. Let $\overline{H}(x, y, t) = H(x, y, t) - \frac{1}{V(M)}$. Then arguing as in Lemma 3.3, we have

$$\frac{\partial}{\partial t}\bar{H}(x,x,t) = -\int_{M} \left|\nabla\bar{H}\right|^{2} \left(x,y,\frac{t}{2}\right) dy$$

Since $\int_M \bar{H}(x, y, t) dy = 0$, the Neumann Sobolev inequality gives

$$\begin{split} &C(S)\int_{M}\left|\nabla\bar{H}\right|^{2}\left(x,y,\frac{t}{2}\right)dy\geq\left(\int_{M}\left|\bar{H}\right|^{\frac{2n}{n-2}}\left(x,y,\frac{t}{2}\right)dy\right)^{\frac{n-2}{n}}\\ &\geq\left(\int_{M}\left|\bar{H}\right|^{2}\left(x,y,\frac{t}{2}\right)dy\right)^{\frac{n+2}{n}}\left(\int_{M}\left|\bar{H}\right|\left(x,y,\frac{t}{2}\right)dy\right)^{-\frac{4}{n}}\\ &=\left(\bar{H}(x,x,t)\right)^{\frac{n+2}{n}}\left(\int_{M}\left|\bar{H}\right|\left(x,y,\frac{t}{2}\right)dy\right)^{-\frac{4}{n}}, \end{split}$$

where we have used the Hölder inequality. But

$$\int_{M} \left| \bar{H} \right| \left(x, y, \frac{t}{2} \right) dy \leq \int_{M} \left(H\left(x, y, \frac{t}{2} \right) + \frac{1}{V(M)} \right) dy \leq 2.$$

Hence

$$\int_{M} \left| \nabla \bar{H} \right|^{2} \left(x, y, \frac{t}{2} \right) dy \ge 2^{-\frac{4}{n}} C^{-1}(S) \left(\bar{H}(x, x, t) \right)^{\frac{n+2}{n}}.$$

In conclusion,

$$\frac{\partial}{\partial t}\bar{H}(x,x,t) \leq -2^{-\frac{4}{n}}C^{-1}(S)\left(\bar{H}(x,x,t)\right)^{\frac{n+2}{n}}$$

Integrating this differntial inequality from $\varepsilon > 0$ to t gives

$$(\bar{H}(x,x,t))^{-\frac{2}{n}} - (\bar{H}(x,x,\varepsilon))^{-\frac{2}{n}} \ge \frac{2}{n} \left(2^{-\frac{4}{n}}C^{-1}(S)\right)(t-\varepsilon).$$

Letting ε tend to 0 and noting that

$$\lim_{\varepsilon \to 0} \left(\bar{H}(x, x, \varepsilon) \right)^{-\frac{2}{n}} = 0,$$

we obtain

$$\bar{H}(x,x,t) \le c(n)(C(S))^{\frac{n}{2}}t^{-\frac{n}{2}}.$$

Using the semi-group property of $\overline{H}(x, y, t)$, we conclude

$$\begin{split} \left| \bar{H}(x,y,2t) \right| &= \left| \int_{M} \bar{H}(x,z,t) \bar{H}(z,y,t) dz \right| \\ &\leq \left(\int_{M} \bar{H}^{2}(x,z,t) dz \right)^{\frac{1}{2}} \left(\int_{M} \bar{H}^{2}(z,y,t) dz \right)^{\frac{1}{2}} \\ &= \bar{H}^{\frac{1}{2}}(x,x,2t) \bar{H}^{\frac{1}{2}}(y,y,2t). \end{split}$$

Therefore, putting the preceding inequalities together, we get

$$\left|\bar{H}(x,y,t)\right| \le c(n)(C(S))^{\frac{n}{2}}t^{-\frac{n}{2}}.$$

Now the theorem follows from Theorem 3.7 and the definition of $\overline{H}(x, y, t)$.

Finally, we mention a corollary on estimating the Neumann eigenvalues. It can be easily proved by using the heat kernel estimates. **Corollary 3.9.** Let M be as in Theorem 3.1. Then the k-th Neumann eigenvalue μ_k of M satisfies

$$\mu_k \ge C_{11}(K, H, V, R, d)k^{\frac{2}{n}}$$

for all $k = 0, 1, 2, \ldots$

4. Parabolic Harnack Inequality.

In this section, we turn to consider the validity of a version of parabolic Harnack inequality on a general complete Riemannian manifold. We shall show the validity of such a parabolic Harnack inequality is equivalent to the existence of Gaussian upper and lower bounds on the heat kernel. Previously, Saloff-Coste [SC] and Grigor'yan [G] had obtained another type of characterization for the parabolic Harnack inequality. To recall their results, let us first introduce some definitions.

Definition 4.1. Let (M, g) be a complete Riemannian manifold. Then (M, g) is said to satisfy the parabolic Harnack inequality (PHI) on balls of radius r_0 if there exists a constant C depending only on the parameters $0 < \varepsilon < \eta < \delta < 1$, such that, for any $x \in M$, and real s, and any $0 < r < r_0$, any nonnegative solution u of $\left(\Delta - \frac{\partial}{\partial t}\right)u = 0$ in $Q = (s - r^2, s) \times B_x(r)$ satisfies

$$\sup_{Q_-} \{u\} \le C \inf_{Q_+} \{u\}$$

where

$$Q_{-} = [s - \delta r^2, s - \eta r^2] \times B_x(\delta r)$$

and

$$Q_+ = [s - \varepsilon r^2, s] \times B_x(\delta r).$$

Definition 4.2. M satisfies volume doubling property on balls of radius r_0 if there exists constant C such that

 $V_x(2r) \le CV_x(r)$ for any $0 < r < r_0$ and $x \in M$,

where $V_x(r)$ denotes the volume of the geodesic ball $B_x(r)$ in M.

Definition 4.3. M satisfies weak-Neumann Poincaré inequality on balls of radius r_0 if there exists a constant C such that

$$\inf_{\alpha \in \mathbf{R}} \int_{B_x(r)} |f - \alpha|^2 d\mu \le Cr^2 \int_{B_x(2r)} |\nabla f|^2 d\mu$$

for any $0 < r < r_0, x \in M$ and $f \in C^{\infty}(M)$.

The following theorem is a special form of the more general results proved independently by Saloff-Coste [SC] and Grigor'yan [G].

Theorem 4.4.

- (a) M satisfies (PHI) on balls of radius r₀ if M satisfies both volume doubling property and weak-Neumann Poincaré inequality on balls of radius 4r₀.
- (b) M satisfies both volume doubling property and weak-Neumann Poincaré inequality on balls of radius r₀ if M satisfies (PHI) on balls of radius 2r₀.

For a general complete manifold, it is well-known that there exists a minimal heat kernel H(x, y, t). We have the following result.

Theorem 4.5.

(a) If M satisfies (PHI) on balls of radius r_0 , then there exist some constants C_1, C_2, C_3 and C_4 such that

$$C_1 V_x^{-1} \left(\sqrt{t}\right) \exp\left(-\frac{r^2(x,y)}{C_2 t}\right) \le H(x,y,t)$$
$$\le C_3 V_x^{-1} \left(\sqrt{t}\right) \exp\left(-\frac{r^2(x,y)}{C_4 t}\right)$$

for any x, y and t such that $r(x, y) \leq r_1 < \frac{r_0}{2}$ and $t < r_1^2$, where r(x, y) denotes the distance between x and y.

(b) If there exist some constants C_1, C_2, C_3 and C_4 such that

$$C_1 V_x^{-1} \left(\sqrt{t}\right) \exp\left(-\frac{r^2(x,y)}{C_2 t}\right) \le H(x,y,t)$$
$$\le C_3 V_x^{-1} \left(\sqrt{t}\right) \exp\left(-\frac{r^2(x,y)}{C_4 t}\right)$$

for any x, y and t such that $r(x, y) \leq r_0$ and $t \leq r_0^2$, then M satisfies (PHI) on balls of radius r_1 for any $r_1 < \frac{r_0}{8}$.

Corollary 4.6. *M* satisfies (PHI) if and only if there exist some constants C_1, C_2, C_3 and C_4 such that

$$C_1 V_x^{-1}\left(\sqrt{t}\right) \exp\left(-\frac{r^2(x,y)}{C_2 t}\right) \le H(x,y,t) \le C_3 V_x^{-1}\left(\sqrt{t}\right) \exp\left(-\frac{r^2(x,y)}{C_4 t}\right)$$

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for any $(x, y, t) \in M \times M \times (0, \infty)$, where r(x, y) denotes the distance between x and y.

Proof of Theorem 4.5. We first show that the validity of (PHI) on balls of radius r_0 implies the heat kernel bounds. Since by Theorem 4.4, M satisfies volume doubling property on balls of radius $\frac{r_0}{2}$, the argument of P. Li and S.T. Yau [L-Y] then implies

$$H(x, y, t) \le C_3 V_x^{-1}\left(\sqrt{t}\right) \exp\left(-\frac{r^2(x, y)}{C_4 t}\right),$$

for any x, y and t such that $r(x, y) \leq r_1 < \frac{r_0}{2}$ and $t < r_1^2$, where C_3 and C_4 are constants depending on r_1 . To establish the desired lower bound of H(x, y, t), for any $x \in M$ and $r \leq r_1 < r_0$, we consider the function defined by $u(z, s) = \int_{B_x(r)} H(y, z, s) dy$ when s > 0 and u(z, s) = 1 when $s \leq 0$. This function is a nonnegative solution of $(\Delta - \frac{\partial}{\partial t})u = 0$ on $B_x(r) \times (-\infty, +\infty)$. Hence we have

$$1 = u(x, -r^2/4) \le Cu(x, r^2/2)$$

= $C \int_{B_x(r)} H(y, x, r^2/2) dy \le C^2 V_x(r) H(x, x, r^2).$

Therefore,

(4.13)
$$H(x, x, r^2) \ge CV_x^{-1}(r)$$

Using the Harnack inequality and the volume doubling property, one easily sees from (4.13) that

$$H(x, y, t) \ge CV_x^{-1}(\sqrt{t})$$
 for $r(x, y) \le \sqrt{t} \le r_1 < r_0$ and $t > 0$,

where C is a constant.

For arbitrary $x, y \in M$ with $r(x, y) \leq r_1 < r_0/2$ and $t \leq r_1^2$, there exists a positive integer $N \geq 1$ such that $N-1 < \frac{4r^2(x, y)}{t} \leq N$. Let $\gamma(t)$ be a minimal geodesic connecting x and y which is parametrized by the arclength. Let $q_i = \gamma\left(\frac{ir(x, y)}{N}\right)$, $i = 0, \ldots, N$. Then by the semi-group property of H(x, y, t), we get

 $(4.15) \\ H(x, y, t)$

$$= \int_{M} \dots \int_{M} H\left(x, z_{1}, \frac{t}{N}\right) H\left(z_{1}, z_{2}, \frac{t}{N}\right) \dots H\left(z_{N-1}, y, \frac{t}{N}\right) dz_{1} \dots dz_{N-1}$$

$$\geq \int_{B_{q_{N-1}}\left(\frac{r}{N}\right)} \dots \int_{B_{q_{1}}\left(\frac{r}{N}\right)} H\left(x, z_{1}, \frac{t}{N}\right) \dots H\left(z_{N-1}, y, \frac{t}{N}\right) dz_{1} \dots dz_{N-1}.$$

For $z_1 \in B_{q_1}\left(\frac{r}{N}\right)$, $r(x, z_1) \leq r(x, q_1) + r(q_1, z_1) \leq \frac{2r}{N}$. But $\frac{4r^2}{t} \leq N$. Therefore $r(x, z_1) \leq \sqrt{\frac{t}{N}}$ and by (4.14) $H\left(x, z_1, \frac{t}{N}\right) \geq CV_x^{-1}\left(\sqrt{\frac{t}{N}}\right)$. Similarly, for $z_{i-1} \in B_{q_{i-1}}\left(\frac{r}{N}\right)$ and $z_i \in B_{q_i}\left(\frac{r}{N}\right)$, we have

$$H\left(z_{i-1}, z_i, \frac{t}{N}\right) \ge CV_{q_{i-1}}^{-1}\left(2\sqrt{\frac{t}{N}}\right), \qquad i = 2, \dots, N-1.$$

Hence by (4.15),

$$(4.16) \quad H(x,y,t) \geq C^{N-1}V_x^{-1}\left(\sqrt{\frac{t}{N}}\right)V_{q_1}^{-1}\left(2\sqrt{\frac{t}{N}}\right)\dots V_{q_{N-1}}^{-1}\left(2\sqrt{\frac{t}{N}}\right)$$
$$\cdot V_{q_1}\left(\frac{r}{N}\right)\dots V_{q_{N-1}}\left(\frac{r}{N}\right).$$

By the volume doubling property,

$$\frac{V_{q_i}(\frac{r}{N})}{V_{q_i}\left(2\sqrt{\frac{t}{N}}\right)} \geq \frac{V_{q_i}(\frac{r}{N})}{V_{q_i}(\frac{4r}{N})} \geq C_5, \quad \text{a constant.}$$

Putting into (4.16), one concludes that

$$H(x, y, t) \ge C^{N-1}C_5^{N-1}V_x^{-1}\left(\sqrt{\frac{t}{N}}\right)$$
$$\ge C_6^{N-1}V_x^{-1}\left(\sqrt{t}\right)$$
$$\ge C_7V_x^{-1}\left(\sqrt{t}\right)\exp(-C_8N)$$
$$\ge C_9V_x^{-1}\left(\sqrt{t}\right)\exp\left(-\frac{r^2(x, y)}{C_{10}t}\right).$$

Therefore part (a) of the theorem is proved.

Now we come to prove part (b) of Theorem 4.5. In view of Theorem 4.4, we need only to check that M satisfies volume doubling property and

weak-Neumann Poincaré inequality on balls of radius $r_0/2$. For any x and $t \leq r_0^2/2$, by the semi-group property of H(x, y, t),

$$\begin{split} C_3 V_x^{-1} \left(\sqrt{2t} \right) &\geq H(x, x, 2t) = \int_M H^2(x, y, t) dy \\ &\geq \int_{B_x(\sqrt{t})} C_1^2 V_x^{-2} \left(\sqrt{t} \right) \exp\left(-\frac{1}{C_2} \right) dy \\ &\geq C V_x^{-1} \left(\sqrt{t} \right) \quad \text{ for some } \ C > 0. \end{split}$$

Thus $V_x(\sqrt{2t}) \leq \tilde{C}V_x(\sqrt{t})$ for all $0 < t < r_0/\sqrt{2}$, where \tilde{C} is a constant. Therefore $V_x(2r) \leq \tilde{C}V_x(\sqrt{2}r) \leq \tilde{C}^2V_x(r)$ for all $r \leq r_0/2$, and M satisfies volume doubling property on balls of radius $r_0/2$.

To show that M satisfies weak-Neumann Poincaré inequality on balls of radius $r_0/2$, we first establish the following claim.

Claim. For any $p \in M$ and $R \leq r_0/2$, there exist constants C_1, C_2 and C_3 independent of p and R such that

$$H_R(x, y, C_1 R^2) \ge C_3 V_n^{-1}(R)$$

for all x and y satisfying

$$r(p,x) \le C_2 R, \quad r(p,y) \le C_2 R,$$

where $H_R(x, y, t)$ is the heat kernel of $B_p(R)$ satisfying the Dirichlet boundary condition.

Once the claim is established, then by an argument of Fabes and Stroock [F-S], one concludes that M satisfies the weak-Neumann Poincaré inequality on balls of radius $r_0/2$.

To check the claim, by the maximum principle, we have

$$H_R(x, y, t) \ge H(x, y, t) - \max_{\substack{0 \le s \le t \\ z \in S_p(R)}} H(x, z, s).$$

From the assumption, there exists a constant C such that for $t \leq r_0^2$,

$$\max_{0 \le s \le t \atop z \in S_p(R)} H(x, z, s) \le \max_{0 \le s \le t} CV_x^{-1}\left(\sqrt{s}\right) \exp\left(-\frac{R^2}{Cs}\right)$$

for all x such that $r(p, x) \leq C_2 R$, $C_2 \leq \frac{1}{2}$. Thus

$$(4.17) \quad \max_{0 \le s \le t \ z \in S_p(R)} H(x, z, s) \le CV_x^{-1}\left(\sqrt{t}\right) \max_{0 \le s \le t} \frac{V_x\left(\sqrt{t}\right)}{V_x\left(\sqrt{s}\right)} \exp\left(-\frac{R^2}{Cs}\right).$$

Since M satisfies volume doubling property on balls of radius $r_0/2$, for some constant $\alpha > 0$ and constant C > 0, $\frac{V_x\left(\sqrt{t}\right)}{V_x\left(\sqrt{s}\right)} \leq C\left(\frac{\sqrt{t}}{\sqrt{s}}\right)^{\alpha}$ (see [G]) for all $\sqrt{s} \leq \sqrt{t} \leq r_0/2$. In particular, (4.17) implies that

$$\max_{\substack{0 \le s \le t \\ x \in S_p(R)}} H(x, z, s)$$

$$\leq CV_x^{-1} \left(\sqrt{t}\right) \max_{0 \le s \le t} \left(\frac{t}{s}\right)^{\alpha} \exp\left(-\frac{R^2}{Cs}\right)$$

$$\leq C_3 V_x^{-1} \left(\sqrt{t}\right) \exp\left(-\frac{R^2}{C_4 t}\right)$$

if $t \leq C_5 R^2$ for some $C_5 > 0$. Thus, for all $t \leq C_5 R^2$,

(4.18)
$$H_R(x, y, t)$$

$$\geq C_1 V_x^{-1} \left(\sqrt{t}\right) \exp\left(-\frac{r^2(x, y)}{C_2 t}\right) - C_3 V_x^{-1} \left(\sqrt{t}\right) \exp\left(-\frac{R^2}{C_4 t}\right).$$

If we choose C_6 sufficiently small such that

$$r(p,x) \le C_6 R$$
 and $r(p,y) \le C_6 R$,

then $r(x, y) \leq 2C_6 R$ and

(4.19)
$$C_3 \exp\left(-\frac{R^2}{C_4 t}\right) \le \frac{1}{2} C_1 \exp\left(-\frac{r^2(x,y)}{C_2 t}\right)$$
 for all $t \le C_5 R^2$.

Together (4.18) and (4.19), we have

$$H_R(x, y, t) \ge CV_x^{-1}\left(\sqrt{t}\right) \exp\left(-\frac{r^2(x, y)}{Ct}\right)$$

for some C > 0 and all $t \leq C_5 R^2$, where $r(p, x) \leq C_6 R$ and $r(p, y) \leq C_6 R$. But

$$V_x^{-1}\left(\sqrt{t}\right) \ge V_p^{-1}\left(\sqrt{t} + r(p,x)\right) \ge V_p^{-1}(2R) \ge CV_p^{-1}(R)$$

by the volume doubling property. Therefore

(4.20)
$$H_R(x, y, t) \ge CV_p^{-1}(R) \exp\left(-\frac{r^2(x, y)}{Ct}\right)$$

for $t \leq C_5 R^2$ and $r(p, x) \leq C_6 R$, $r(p, y) \leq C_6 R$. In particular, let $t = C_5 R^2$ in (4.20), the claim follows. This completes our proof of Theorem 4.5.

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