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HEAT KERNEL REMAINDERS AND INVERSE SPECTRAL THEORY

BY

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1. Introduction

Suppose that $\mathscr{D}$ denotes a relatively compact domain, with smooth boundary, in a complete Riemannian manifold M^n. If one imposes Dirichlet boundary conditions, then the Laplacian Δ defines a self adjoint operator in $L^2\mathscr{D}$. The associated heat operator $\exp(t\Delta)$ is given by a smoothing kernel $E_{\mathscr{D}}(t, x, y)$, for $x, y \in \mathscr{D}$. Elementary parabolic theory determines the asymptotic behavior, as $t \downarrow 0$, of the remainder

$$h_{\mathscr{D}}(t) = |(4\pi t)^{n/2} \operatorname{Tr} E_{\mathscr{D}}(t) - \operatorname{vol} \mathscr{D}|.$$

In particular, we have $h_{\mathscr{D}}(t)$ of order $t^{1/2}$. However, the basic theory does not provide good geometric control in this order estimate.

Our first goal is to obtain bounds of the form $h_{\mathscr{D}}(t) \leq \hat{h}_{\mathscr{D}}(t)$, valid for all $t > 0$. The function $\hat{h}_{\mathscr{D}}(t)$ will be given in terms of specific elementary functions of t, and will satisfy $\hat{h}_{\mathscr{D}}(t) = O(t^{1/2})$, as $t \downarrow 0$. The key point is that the bound $\hat{h}_{\mathscr{D}}(t)$ shall have precise geometric dependence. If $M = R^n$, the n-dimensional Euclidean space, and $\mathscr{D}$ is convex, then this problem was studied earlier by Angelescu, Nenciu, and van den Berg, [1], [2]. They showed that, for this special case, $\hat{h}_{\mathscr{D}}(t)$ need only depend upon $\operatorname{vol}(\partial\mathscr{D})$, the $n - 1$ dimensional volume of $\partial\mathscr{D}$. Their work has applications in quantum statistical mechanics.

If M is simply connected and negatively curved, then we prove, in Theorem 2.5, that $\hat{h}_{\mathscr{D}}(t)$ need only depend upon $\operatorname{vol}(\partial\mathscr{D})$, a lower bound for the Ricci curvature of $\mathscr{D}$, $\operatorname{vol}(\mathscr{D})$, and an upper bound for the mean curvature of $\partial\mathscr{D}$, with respect to an inward pointing normal. In particular, one does not necessarily assume that $\mathscr{D}$ is convex. For dimension $n = 2$, we remove any assumption about the curvature of $\partial\mathscr{D}$. On general complete M, one determines $\hat{h}_{\mathscr{D}}(t)$ using in addition an upper bound for the sectional curvature and a lower bound for the injectivity radius, on a proper neighborhood of $\mathscr{D}$. This is done in Theorem 3.5, our principal general result. Again,

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all hypotheses on the curvature of the boundary, $\partial\mathscr{D}$, can be dropped for $n = 2$. The heat kernel estimates of Sections 2 and 3 are developed from earlier work by the first author and Li [7].

In our final Section 4, we apply our heat kernel remainder estimates to a question of inverse spectral theory. The asymptotic formula of Weyl shows that knowledge of all the eigenvalues $-\lambda_i$, $1 \le i < \infty$, of Δ acting on $L^2\mathscr{D}$ with Dirichlet boundary data, determines $\mathrm{vol}(\mathscr{D})$. One naturally asks how many eigenvalues $-\lambda_i$, $1 \le i \le N$, are needed to find $\mathrm{vol}(\mathscr{D})$ up to a given error ε. Li and Yau [11] answered this question for convex domains in R^n. The second author, of the present paper, extended their work to convex domains in complete spaces with constant negative curvature [10]. Since Li and Yau rely upon a rather delicate subdivision into cubes and minimax comparison, it seems onerous to develop their approach for M of variable curvature. Our heat kernel method appears to be more flexible. We obtain results for convex domains in quite general Riemannian manifolds M. The precise statement of our conclusions, for approximating $\mathrm{vol}(\mathscr{D})$ by finitely many λ_i, appear as Theorem 4.3. Again, the key point is to have good geometric control of the relevant error estimate. One requires certain information about the ambient manifold M. The only hypothesis specific to $\mathscr{D}$ is that $\mathscr{D}$ is convex.

Throughout the paper we use the Greek letters α_i, β_i to denote universal numerical constants. In particular, these constants do not depend upon the geometry of M or $\mathscr{D}$.

2. Heat kernels-simply connected spaces with negative curvatures

Suppose that M^n is a simply connected complete space with negative sectional curvatures. By a theorem of Hadamard-Cartan, the geodesic distance r defines a smooth function r^2. This globally defined r^2 is very helpful for deriving heat kernel estimates. Let $\mathscr{D}$ be a relatively compact domain, with smooth boundary $\partial\mathscr{D}$, contained in the given manifold M. Our goal is to obtain upper bounds, with precise geometric dependence, for the remainder

$$|\mathrm{Tr}\, E_{\mathscr{D}}(t) - (4\pi t)^{-n/2}\mathrm{vol}\,\mathscr{D}|.$$

Additional hypotheses will eventually be imposed upon $\mathscr{D}$ and M.

As usual, $E_{\mathscr{D}}(t, x, y)$ denotes the heat kernel for $\mathscr{D}$ with Dirichlet boundary conditions. One has the elementary upper bound:

PROPOSITION 2.1. *$E_{\mathscr{D}}(t, x, x) \le (4\pi t)^{-n/2}$ for all $x \in \mathscr{D}$.*

Proof. This follows from a standard heat kernel comparison [6]. Since we employ this method repeatedly, a sketch is included.

Let $E_0(t, x, y) = (4\pi t)^{-n/2} \exp(-r^2(x, y)/4t)$ be the transplant of a Euclidean heat kernel, where r is the geodesic distance of M. One calculates

$$\left(\Delta_y - \frac{\partial}{\partial t}\right) E_0(t, x, y) = \left(\frac{\partial^2}{\partial r^2} + \left(\frac{\theta'}{\theta} + \frac{n-1}{r}\right)\frac{\partial}{\partial r} - \frac{\partial}{\partial t}\right) E_0(t, x, y)$$
$$= \frac{\theta'}{\theta}\frac{\partial}{\partial r} E_0(t, x, y).$$

Here θ is the Jacobian determinant of the exponential map $\exp: T_x M \to M$. Since the sectional curvatures of M are negative $\theta'/\theta = \partial/\partial r(\log \theta) \geq 0$. Consequently, $E_0(t, x, y)$ is a supersolution of the heat equation problem, $(\Delta - \partial/\partial t)E_0(t, x, y) \leq 0$.

Duhamel's principle states that

$$E_0(t, x, y) - E_{\mathscr{D}}(t, x, y) = \int_0^t \frac{\partial}{\partial s}\left[\int_{\mathscr{D}} E_0(s, x, z) E_{\mathscr{D}}(t - s, z, y)\, dz\right] ds.$$

Since $(\Delta - \partial/\partial t)E = 0$ and $(\Delta - \partial/\partial t)E_0 \leq 0$, this gives

$$E_0(t, x, y) - E_{\mathscr{D}}(t, x, y) \geq \int_0^t \int_{\mathscr{D}} [\Delta E_0(s, x, z) E_{\mathscr{D}}(t - s, z, y)$$
$$- E_0(s, x, z) \Delta E_{\mathscr{D}}(t - s, z, y)]\, dz\, ds.$$

Integrating by parts twice gives

$$E_0(t, x, y) - E_{\mathscr{D}}(t, x, y) \geq \int_0^t \int_{\partial\mathscr{D}} E_0(s, x, z) \frac{\partial}{\partial \nu} E_{\mathscr{D}}(t - s, z, y)\, dz\, ds \geq 0.$$

Here $\partial/\partial\nu$ denotes the inward unit normal derivative. The last integral is positive, since $E_{\mathscr{D}}$ satisfies Dirichlet boundary conditions. Proposition 2.1 follows by setting $x = y$ and recalling the definition of E_0.

We proceed to derive a complementary lower bound for the heat kernel. The argument here is more subtle, since we need a bound which differs from the most basic estimate [4]. Assume now that the Ricci curvature of M is bounded below by $-(n - 1)a$, for some positive a.

It is expedient to prepare our argument via some elementary lemmas. To begin, one has a lower bound for the heat kernel E_{-a}, on a simply connected complete space M_a with constant sectional curvature $-a$.

LEMMA 2.2. *$E_{-a}(t, x, x) \geq (4\pi t)^{-n/2} - \beta_1 a t^{-n/2+1}$ for some positive constant β_1.*

Proof. Since M_a admits a transitive group of isometries, $E_{-a}(t, x, x)$ is independent of $x \in M_a$. If $\gamma > 0$, then $E_{-\gamma_a}(t, x, x)$ is equal to $\gamma^{n/2}E_{-a}(\gamma t, x, x)$. This equality follows by scaling the metric and invoking the uniqueness characterization for the fundamental solution of the heat equation. Choosing $\gamma = a^{-1}$, one reduces to the case $a = 1$. As $t \downarrow 0$, the asymptotic expansion for the heat kernel gives

$$E_{-1}(t, x, x) = (4\pi t)^{-n/2} + O(t^{-n/2+1}).$$

Since the heat kernel is positive, our assertion is clear for large $t \uparrow \infty$. The existence of β_1 now follows from the continuity of $E_{-1}(t, x, x)$.

Let $E_{0,d}(t, x, y)$ be the heat kernel for a ball of radius d in Euclidean space M_0. Of course, Dirichlet boundary conditions are imposed upon $E_{0,d}$. The following fact is well-known [2]:

LEMMA 2.3. *At the center x, of the Euclidean ball with radius d, one has*

$$E_0(t, x, x) - E_{0,d}(t, x, x) \leq \beta_2 t^{-n/2} e^{-\beta_3 d^2/t}.$$

Proof. If α is a suitable positive constant, then the ball of radius d contains a cube of side αd. Duhamel's principle gives $E_{0,d}(t, x, x) \geq \overline{E}_{0,\alpha d}(t, x, x)$, where $\overline{E}$ is the heat kernel of the cube. It therefore suffices to prove the inequality

$$\overline{E}_{0,\alpha d}(t, x, x) \geq (4\pi t)^{-n/2} - \beta_2 t^{-n/2} e^{-\beta_3 d^2/t}$$

since $E_0(t, x, x) = (4\pi t)^{-n/2}$. By scaling, we further reduce to the case $\alpha d = 2$.

Suppose one considers an interval of length two centered at the origin in R^1. Using Duhamel's principle

$$\begin{aligned}\overline{E}_{0,1}(t, z, y) \geq (4\pi t)^{-1/2} &\exp(-|z - y|^2/4t)\\ -(4\pi t)^{-1/2} &\exp(-|z + y - 2|^2/4t)\\ -(4\pi t)^{-1/2} &\exp(-|z + y + 2|^2/4t).\end{aligned}$$

Setting $y = z = 0$, we get the required estimate in one dimension. The n dimensional case follows since the heat kernel of an n-cube is a product of one dimensional kernels.

Employing these lemmas, one can derive a lower bound for the kernel $E_{\mathscr{D}}(t, x, x)$. Let $x \in \mathscr{D}$ be a point whose distance from the boundary $\partial\mathscr{D}$ is $d = d(x)$.

PROPOSITION 2.4. $E_{\mathscr{D}}(t, x, x) \geq (4\pi t)^{-n/2} - \beta_4 e^{\beta_5\sqrt{a}d} t^{-n/2} e^{-\beta_3 d^2/t} - \beta_1 a t^{-n/2+1}$.

Proof. Let B denote the ball of radius $d(x)$ centered at $x \in M$. Since $B \subset \mathscr{D}$, Duhamel's principle yields $E_{\mathscr{D}}(t, x, x) \geq E_B(t, x, x)$. The problem is reduced to the case where our domain is a ball. Duhamel's principle gives

$$E_M(t, x, x) - E_B(t, x, x) = \int_0^t \int_{\partial B} E_M(s, x, y) \frac{\partial}{\partial \nu} E_B(t - s, y, x)\, dy\, ds$$

where $\partial/\partial\nu$ denotes the interior normal derivative.

Suppose that B_0 is a ball with radius d, centered at a point $x_0 \in M_0$, the Euclidean space of dimension n. One has the upper bounds

$$E_M(t, x, y) \leq E_0(t, x, y) \quad \text{and} \quad E_B(t, y, x) \leq E_{0,d}(t, y, x).$$

Here E_0 is the transplant of the Euclidean kernel to M, $E_0(t, x, y) = E_0(t, r(x, y))$. Similarly, $E_{0,d}(t, x, y)$ is a transplant from the ball B_0, obtained by identifying x and x_0. It follows that

$$E_M(t, x, x) - E_B(t, x, x) \leq \int_0^t \int_{\partial B} E_0(s, x, y) \frac{\partial}{\partial \nu} E_{0,d}(t - s, y, x)\, dy\, ds.$$

Using the lower bound on Ricci curvature to obtain an upper bound for the volume element, one finds

$$\begin{aligned} &E_M(t, x, x) - E_B(t, x, x) \\ &\quad \leq \beta_6 \int_0^t \int_{\partial B_0} e^{\beta_5\sqrt{a}d} E_0(s, x_0, z) \frac{\partial}{\partial \nu} E_{0,d}(t - s, z, x_0)\, dz\, ds. \end{aligned}$$

We apply Duhamel's principle to evaluate the integral on the right hand side. This yields

$$E_M(t, x, x) - E_B(t, x, x) \leq \beta_6 e^{\beta_5\sqrt{a}d} (E_0(t, x_0, x_0) - E_{0,d}(t, x_0, x_0)).$$

Invoking Lemma 2.3 gives

$$E_M(t, x, x) - E_B(t, x, x) \leq \beta_4 e^{\beta_5\sqrt{a}d} t^{-n/2} e^{-\beta_3 d^2/t}.$$

Duhamel's principle and the lower bound of Ricci curvature establish $E_M \geq E_{-a}$. Thus, if $x_1 \in M_a$ is arbitrary,

$$E_B(t, x, x) \geq E_{-a}(t, x_1, x_1) - \beta_4 e^{\beta_5\sqrt{a}d} t^{-n/2} e^{-\beta_3 d^2/t}.$$

Proposition 2.4 now follows from Lemma 2.2.

Suppose that $c \geq 0$ is an upper bound for the mean curvature of $\partial\mathscr{D}$, with respect to an inward pointing unit normal. The main result of this section is a remainder estimate:

THEOREM 2.5.

$$\begin{aligned}
&|\operatorname{Tr} E_{\mathscr{D}}(t) - (4\pi t)^{-n/2}\operatorname{vol}\mathscr{D}| \\
&\quad \leq \alpha_1 \frac{1}{\sqrt{at}} \int_0^\infty e^{\alpha_2 s} e^{-\alpha_3 s^2/at}\, ds \left(1 + |\frac{c}{\sqrt{a}}|\right)^{n-1} t^{-n/2+1/2} \operatorname{vol}\partial\mathscr{D} \\
&\qquad + \alpha_4 at\, t^{-n/2} \operatorname{vol}\mathscr{D}.
\end{aligned}$$

Here the α_i are positive constants.

Proof. By integrating the estimate of Proposition 2.1, we get

$$\operatorname{Tr} E_{\mathscr{D}}(t) = \int_{\mathscr{D}} E_{\mathscr{D}}(t,x,x)\, dx \leq (4\pi t)^{-n/2}\operatorname{vol}\mathscr{D}.$$

So $\operatorname{Tr} E_{\mathscr{D}}(t) - (4\pi t)^{-n/2}\operatorname{vol}\mathscr{D} \leq 0$. It remains to give a lower bound for the heat kernel remainder.

To prove this complementary bound, we use the exponential map $\exp{:}\partial\mathscr{D} \times R^+ \to \mathscr{D}$, along an inward pointing unit normal. Let $W \subset \partial\mathscr{D} \times R^+$ be an open neighborhood of $\partial\mathscr{D} \times 0$, so that $\mathscr{D} - \exp W$ has measure zero and $\exp{:}W \to \exp W$ is a diffeomorphism. If $\mathscr{J}(y,u)$ denotes the Jacobian determinant of exp, at $(y,u) \in \partial\mathscr{D} \times R^+$, then

$$\operatorname{Tr} E_{\mathscr{D}}(t) = \int_W E_{\mathscr{D}}(t,x,x)\mathscr{J}(y,u)\, dy\, du$$

where $x = \exp(y,u)$.

From Proposition 2.4, we get

$$\begin{aligned}
\operatorname{Tr} E_{\mathscr{D}}(t) \geq{}& (4\pi t)^{-n/2}\operatorname{vol}\mathscr{D} - \beta_1 at^{-n/2+1}\operatorname{vol}\mathscr{D} \\
&- \beta_4 t^{-n/2} \int_W e^{\beta_5\sqrt{a}u} e^{-\beta_3 u^2/t} \mathscr{J}(y,u)\, dy\, du. \qquad (2.6)
\end{aligned}$$

The comparison theory of [8], gives the bound

$$\mathscr{J}(y,u) \leq \beta_7 e^{\beta_8\sqrt{a}u}\left(1 + \left|\frac{c}{\sqrt{a}}\right|\right)^{n-1}$$

with the immediate consequence

$$\begin{aligned}\operatorname{Tr} E_{\mathscr{D}}(t) - (4\pi t)^{-n/2} \operatorname{vol} \mathscr{D} \geq & -\beta_1 a t^{-n/2+1} \operatorname{vol} \mathscr{D} \\ & - \beta_9 t^{-n/2} \left(\int_0^\infty e^{\beta_{10}\sqrt{a}\, u} e^{-\beta_3 u^2/t}\, du \right) \\ & \times \left(1 + \left| \frac{c}{\sqrt{a}} \right| \right)^{n-1} \operatorname{vol} \partial\mathscr{D}.\end{aligned}$$

Theorem 2.5 follows after making the change of variable $s = \sqrt{a}\, u$ in the integral.

In the two dimensional case, a variation of our method allows one to remove any assumption about the curvature of the boundary $\partial\mathscr{D}$. Let $\chi(\mathscr{D})$ denote the Euler characteristic of our domain $\mathscr{D}$. One has:

THEOREM 2.7. *If $n = \dim M = 2$, then*

$$\begin{aligned}\left| \operatorname{Tr} E_{\mathscr{D}}(t) - (4\pi t)^{-1} \operatorname{vol} \mathscr{D} \right| \leq & \frac{\alpha_5}{\sqrt{at}} \left(\int_0^\infty e^{\alpha_6 s} e^{-\alpha_7 s^2/at}\, ds \right) t^{-1/2} \operatorname{vol} \partial\mathscr{D} \\ & + \alpha_8 |\chi(\mathscr{D})| \frac{1}{at} \left(\int_0^\infty s e^{\alpha_6 s} e^{-\alpha_7 s^2/at}\, ds \right) \\ & + \alpha_9 a \operatorname{vol} \mathscr{D}.\end{aligned}$$

Proof. We follow the proof of Theorem 2.5, with $n = 2$, verbatim until we reach formula (2.6). Let $W(u)$ be the $n - 1$ dimensional slice of W, where the second coordinate u is fixed. Define

$$L(u) = \int_{W(u)} \mathscr{J}(y, u)\, dy.$$

According to (2.6) and Fubini's theorem

$$\begin{aligned}& \operatorname{Tr} E_{\mathscr{D}}(t) - (4\pi t)^{-1} \operatorname{vol} \mathscr{D} \\ & \quad \geq -\beta_1 a \operatorname{vol} \mathscr{D} - \beta_4 t^{-1} \int_0^\infty e^{\beta_5 \sqrt{a}\, u} e^{-\beta_3 u^2/t} L(u)\, du.\end{aligned}$$

From [3] and [9], one has the remarkable upper bound $L(u) \leq \operatorname{vol} \partial\mathscr{D} + 2\pi|\chi(\mathscr{D})|u$. The key point is that this estimate requires no hypotheses about the curvature of $\partial\mathscr{D}$.

Substitution yields

$$\begin{aligned}
\operatorname{Tr} E_{\mathscr{D}}(t) &- (4\pi t)^{-1}\operatorname{vol}\mathscr{D} \\
&\geq -\beta_1 a \operatorname{vol}\mathscr{D} - \beta_4 \operatorname{vol}(\partial\mathscr{D}) t^{-1} \int_0^\infty e^{\beta_5\sqrt{a}u} e^{-\beta_3 u^2/t}\, du \\
&\quad - \beta_4 2\pi |\chi(\mathscr{D})| t^{-1} \int_0^\infty u e^{\beta_5\sqrt{a}u} e^{-\beta_3 u^2/t}\, du.
\end{aligned}$$

Theorem 2.7 now follows from setting $s = \sqrt{a}\, u$ in each integral.

3. Heat kernels-general Riemannian manifolds

Let $\mathscr{D}$ be a relatively compact domain, with smooth boundary, in a complete Riemannian manifold M. Suppose that $I_{\mathscr{D}}$ is a finite positive number so that, for each $p \in \mathscr{D}$, the exponential map $\exp: B(p, I_{\mathscr{D}}) \to M$ is a diffeomorphism. Here $B(p, I_{\mathscr{D}})$ denotes a ball of radius $I_{\mathscr{D}}$ in the tangent space to M at p. Let $D' = \bigcup_{p \in \mathscr{D}} \exp B(p, I_{\mathscr{D}})$. Then $\mathscr{D}'$ is a relatively compact open set containing $\mathscr{D}$. Choose an upper bound b for the sectional curvatures of M at points in $\mathscr{D}'$. Set $I = \min(I_{\mathscr{D}}, \pi/\sqrt{b})$. Assume that $-(n-1)a$ is a lower bound for the Ricci curvature of M at points in $\mathscr{D}$.

Our purpose is to generalize the results from Section 2. The first step is to extend the preliminary work on upper and lower bounds for the heat kernel. Let E_b denote the heat kernel of the sphere S^n with constant curvature b. One has:

LEMMA 3.1. $E_b(t, x, x) \leq (4\pi t)^{-n/2} + \beta_1 b t^{-n/2+1} + \beta_2 b^{n/2+1} t.$

Proof. Since S^n admits a transitive group of isometries, the diagonal restriction of the heat kernel, $E_b(t, x, x)$, is independent of x. If one scales the metric and notes the uniqueness property of the heat kernel, one has $E_{\gamma b}(t, x, x) = \gamma^{n/2} E_b(\gamma t, x, x)$, for all $\gamma > 0$. We reduce our task to establishing the lemma when $b = 1$, simply by setting $\gamma = b^{-1}$. The asymptotic expansion of Minakshisundaram-Pleijel guarantees that

$$E_1(t, x, x) = (4\pi t)^{-n/2} + O(t^{-n/2+1}) \quad \text{as } t \downarrow 0.$$

For large t, the kernel $E_1(t, x, x)$ decays to a constant. Lemma 3.1 follows from the continuity of $E_1(t, x, x)$.

Let $E_{\mathscr{D}}(t, x, y)$ denote the heat kernel of $\mathscr{D}$, where one imposes Dirichlet boundary conditions. If x is sufficiently close to y, we transplant $E_b(t, x, y)$ to $\mathscr{D}$, as a function of the geodesic distance. This transplanted kernel is then defined on some neighborhood of the diagonal in $\mathscr{D} \times \mathscr{D}$. The crucial lemma required for the upper bound of $E_{\mathscr{D}}$ is:

LEMMA 3.2. *$E_{\mathscr{D}}(t, x, x) \leq E_b(t, x, x) + d_0 t$. Here the constant d_0 depends upon b and I.*

Proof. This result was established in [7]. The idea of the proof is to construct a supersolution for the heat equation problem of $\mathscr{D}$ with Dirichlet boundary conditions. If $\rho(x, y)$ is an appropriate cut-off function, then a calculation verifies that $(\Delta - \partial/\partial t)(\rho(x, y)E_b(t, x, y))$ is bounded above by a positive constant. Thus, for suitable d_0, $\rho(x, y)E_b(t, x, y) + d_0 t$ is a supersolution. Lemma 3.2 then follows from Duhamel's principle.

Combining the two previous lemmas, one immediately deduces:

PROPOSITION 3.3. *$E_{\mathscr{D}}(t, x, x) \leq (4\pi t)^{-n/2} + \beta_1 b t^{-n/2+1} + dt$. The constant d depends only upon b and I.*

The complementary lower bound can be quickly dispatched. Let $x \in \mathscr{D}$ be a point of distance $r(x)$ from the boundary of $\mathscr{D}$. We may write

PROPOSITION 3.4. *$E_{\mathscr{D}}(t, x, x) \geq (4\pi t)^{-n/2} - \beta_3 e^{\beta_4 \sqrt{a} r} e^{-\beta_5 r^2/t} t^{-n/2} - \beta_6 a t^{-n/2+1}$.*

Proof. In their paper [4], Cheeger and Yau proved a remarkable lower bound,

$$E_{\mathscr{D}}(t, x, x) \geq E_{-a, r}(t, x, x).$$

Here $E_{-a, r}$ is the transplant of the Dirichlet heat kernel on a ball of radius r in the simply connected complete space M_{-a} having constant sectional curvature $-a$. The notable point is that r need not be less than the injectivity radius at $x \in M$.

It now suffices to prove the required lower bound in the special case where $\mathscr{D}$ is a ball of radius r in M_{-a}. This is achieved simply by quoting Proposition 2.4.

Let $c \geq 0$ be an upper bound for the mean curvature of $\partial\mathscr{D}$, with respect to an inward pointing unit normal. Our principal general result is

THEOREM 3.5.

$$\begin{aligned}
&|\operatorname{Tr} E_{\mathscr{D}}(t) - (4\pi t)^{-n/2} \operatorname{vol} \mathscr{D}| \\
&\quad \leq \alpha_1 \frac{1}{\sqrt{at}} \int_0^\infty e^{\alpha_2 s} e^{-\alpha_3 s^2/at}\, ds \left(1 + \left|\frac{c}{\sqrt{a}}\right|\right)^{n-1} t^{-n/2+1/2} \operatorname{vol} \partial\mathscr{D} \\
&\qquad + \alpha_4 (a + b) t t^{-n/2} \operatorname{vol}(\mathscr{D}) + dt \operatorname{vol} \mathscr{D}.
\end{aligned}$$

Proof. One may integrate the upper bound of Proposition 3.3 to get

$$\begin{aligned}\operatorname{Tr} E_{\mathscr{D}}(t) - (4\pi t)^{-n/2}\operatorname{vol}\mathscr{D} &= \int_{\mathscr{D}}\left[E(t,x,x) - (4\pi t)^{-n/2}\right]dx\\ &\le \beta_1 b t^{-n/2+1}\operatorname{vol}\mathscr{D} + dt\operatorname{vol}\mathscr{D}.\end{aligned}$$

It remains to give a lower bound for the remainder $\operatorname{Tr} E_{\mathscr{D}}(t) - (4\pi t)^{-n/2}\operatorname{vol}\mathscr{D}$. For this one follows the analogous part, in the proof of Theorem 2.5, almost verbatim. The only small change is to quote Proposition 3.4 instead of Proposition 2.4.

We now assume that the dimension of $\mathscr{D}$ is two. Again, it is possible to remove any hypothesis about the curvature of the boundary $\partial\mathscr{D}$. If $\chi(\mathscr{D})$ is the Euler characteristic of $\mathscr{D}$, then we may write:

THEOREM 3.6. *If the dimension n is 2, one has*

$$\begin{aligned}&\left|\operatorname{Tr} E_{\mathscr{D}}(t) - \frac{\operatorname{vol}\mathscr{D}}{4\pi t}\right|\\ &\quad\le \frac{\alpha_5}{\sqrt{at}}\left(\int_0^\infty e^{\alpha_6 s}e^{-\alpha_7 s^2/at}\,ds\right)t^{-1/2}\operatorname{vol}(\partial\mathscr{D})\\ &\qquad + \alpha_8(|\chi(\mathscr{D})| + b\operatorname{vol}\mathscr{D})\frac{1}{at}\left(\int_0^\infty s e^{\alpha_6 s}e^{-\alpha_7 s^2/at}\right)ds\\ &\qquad + \alpha_9(a+b)\operatorname{vol}\mathscr{D} + \alpha_{10}\, dt\operatorname{vol}\mathscr{D}.\end{aligned}$$

Proof. The upper bound of $\operatorname{Tr} E_{\mathscr{D}}(t) - (4\pi t)^{-1}\operatorname{vol}\mathscr{D}$ is obtained exactly as in the proof for Theorem 3.5. To bound the heat kernel remainder below, one employs the method from Theorem 2.7. Of course, one again uses Proposition 3.4 as an alternative to Proposition 2.4. More significantly, when quoting [3] and [9], an additional term appears because our sectional curvatures need not be negative. More precisely,

$$L(u) \le \operatorname{vol}(\partial\mathscr{D}) + 2\pi|\chi(\mathscr{D})|u + ub\operatorname{vol}\mathscr{D}.$$

The proof is completed as before.

4. Applications involving eigenvalues

Suppose that $\mathscr{D}$ is a relatively compact domain, with smooth boundary $\partial\mathscr{D}$, in a complete Riemannian manifold M. The Laplacian Δ acts on $L^2\mathscr{D}$, with Dirichlet boundary conditions. According to standard elliptic theory, the operator Δ has pure point spectrum, consisting of eigenvalues $-\lambda_i$, $i \ge 1$. If one knows all of these eigenvalues, then the volume of $\mathscr{D}$ is determined. This follows from the asymptotic formula of Weyl. Li and Yau [11] raised the question of approximating the volume of $\mathscr{D}$ by using a finite number of eigenvalues. The point is to determine how many λ_i are needed to find vol $\mathscr{D}$, to a given accuracy ε. This problem was resolved, by Li and Yau, for convex domains in Euclidean space.

We assume below that $\mathscr{D}$ is a weakly convex domain in M. More precisely, let $p, q \in \partial\mathscr{D}$ be any two points which are joined by a unique minimizing geodesic, denoted γ. Our assumption is that $\gamma \subset \overline{\mathscr{D}}$, the closure of $\mathscr{D}$. Using normal coordinate charts, centered at points $p \in \partial\mathscr{D}$, one sees that the principal curvatures of $\partial\mathscr{D}$ are non-negative, with respect to an outward pointing normal. The boundaries of weakly convex domains may include pairs of points which are not joined by a unique minimizing geodesic.

Our purpose is to extend the results of Li and Yau to weakly convex domains in general Riemannian manifolds. We achieve this goal by relying upon the heat kernel remainder estimates derived earlier in the present paper. The approach of Li and Yau is quite different. It employs careful subdivision into cubes and comparison using the minimax principle. This subdivision approach was developed by the second author, of the current paper, for domains in complete simply connected M of constant negative sectional curvature, [10]. There seem to be serious obstructions hindering the extension of the Li-Yau method to general Riemannian M.

The weak convexity of $\mathscr{D}$ is used essentially in the following

LEMMA 4.1. (i) *If M is compact, then* $\operatorname{vol}(\partial\mathscr{D}) \leq c_1 \operatorname{vol} M$. *Here c_1 depends upon an upper bound for the sectional curvature and a lower bound for the convexity radius of M.*

(ii) *If M is noncompact, assume $\mathscr{D}$ is contained in $B(p, R)$, a geodesic ball of radius R. Then*

$$\operatorname{vol}(\partial\mathscr{D}) \leq c_2 \operatorname{vol} B(p, R+1).$$

The constant c_2 depends upon an upper bound for the sectional curvature and a lower bound for the convexity radius of $B(p, R+1)$.

Proof. Let $\varepsilon_1 < 1$ be a lower bound for the convexity radius. Thus ε_1 is less than the injectivity radius, for all appropriate initial points q, and all geodesic balls $B(q, s)$, $s < \varepsilon_1$, are strongly convex. Here $q \in M$, for case (i), and $q \in B(p, R+1)$, for case (ii). By strongly convex, we mean that if $x_1, x_2 \in \partial B(q, s)$, then x_1 and x_2 are joined by a unique minimizing geodesic, $\gamma \subset M$. Moreover $\gamma - x_1 - x_2 \subset B(q, s)$, the open ball.

Since $\mathscr{D}$ is weakly convex, the principal curvatures of $\partial\mathscr{D}$ are non-negative, with respect to an outward pointing normal. Also, we have an upper bound on the sectional curvatures of M, assuming (i), or the curvatures of $B(p, R+1)$, assuming (ii). For ε_2 depending upon these curvature bounds and if $u < \varepsilon_2 < 1$, then the comparison theorem of Warner [12] guarantees that the Jacobian determinant of exp: $\partial\mathscr{D} \times (0, u) \to M$ is greater than $1/2$, at every point in $\partial\mathscr{D} \times (0, u)$.

Consider the exponential map exp: $\partial\mathscr{D} \times R^+ \to M$, along an outward pointing normal. Suppose $u \in R^+$ is the second coordinate in $\partial\mathscr{D} \times R^+$. If $u < \min(\varepsilon_1, \varepsilon_2)$, then exp: $\partial\mathscr{D} \times (0, u) \to M$ is one to one. This follows easily from the fact that $\mathscr{D}$ is weakly convex and all $B(q, u)$ are strongly convex. Again $q \in M$ for (i), or $q \in B(p, R + 1)$, for (ii).

Assume $u < \min(\varepsilon_1, \varepsilon_2)$. By combining the above results, we see that

$$\exp\colon \partial\mathscr{D} \times (0, u) \to M$$

is 1-1 with Jacobian determinant bounded below by $1/2$. Thus

$$\tfrac{1}{2}\operatorname{vol}(\partial\mathscr{D})\min(\varepsilon_1, \varepsilon_2) \le \operatorname{vol} M,$$

in case (i). For (ii), we similarly deduce

$$\tfrac{1}{2}\operatorname{vol}(\partial\mathscr{D})\min(\varepsilon_1, \varepsilon_2) \le \operatorname{vol} B(p, R + 1).$$

LEMMA 4.2. *Let $\varepsilon > 0$ be given. Then for δ sufficiently small and for all $0 < t \le \delta$, one has*

$$|(4\pi t)^{n/2}\operatorname{Tr} E_{\mathscr{D}}(t) - \operatorname{vol}\mathscr{D}| < c_3 t^{1/2} < \varepsilon/2.$$

Here $\operatorname{Tr} E_{\mathscr{D}}(t) = \int_{\mathscr{D}} E_{\mathscr{D}}(t, x, x)\, dx$ *is the trace of the heat kernel for Dirichlet boundary data.*

Moreover:

(i) If M is compact, then δ and c_3 depend upon an upper bound for the volume and the sectional curvature of M, a lower bound for the Ricci curvature of M, and a lower bound for the convexity radius of M.

(ii) If M is noncompact, assume $\mathscr{D}$ is contained in a ball $B(p, R)$. Then δ and c_3 depend upon R, an upper bound for the sectional curvatures of $B(p, R + 1)$, a lower bound for the convexity radius of $B(p, R + 1)$ and a lower bound for the Ricci curvatures of $B(p, R + 1)$.

Proof. If ε_3 is less than the convexity radius at $q \in M$, then by definition the exponential map $\exp\colon B_0(q, \varepsilon_3) \to B(q, \varepsilon_3)$ is a diffeomorphism. Moreover, the image is strongly convex. Of course, $B_0(q, \varepsilon_3)$ denotes a ball centered at the origin in the tangent space T_qM.

Since $\mathscr{D}$ is weakly convex, we may apply Theorem 3.5, with $c = 0$. This reads

$$|(4\pi t)^{n/2}\operatorname{Tr} E_{\mathscr{D}}(t) - \operatorname{vol}\mathscr{D}| \le \alpha_1 \frac{1}{\sqrt{at}}\left(\int_0^\infty e^{\alpha_2 s} e^{-\alpha_3 s^2/at}\,ds\right) t^{1/2}\operatorname{vol}(\partial\mathscr{D}) + \alpha_4(a+b)t\operatorname{vol}(\mathscr{D}) + dt\operatorname{vol}(\mathscr{D})t^{n/2}.$$

Assume we are in case (i), where M is compact. Obviously $\operatorname{vol}\mathscr{D} \le \operatorname{vol} M$. From Lemma 4.1, $\operatorname{vol}\partial\mathscr{D} \le c_1 \operatorname{vol} M$. So

$$|(4\pi t)^{n/2}\operatorname{Tr} E_{\mathscr{D}}(t) - \operatorname{vol}\mathscr{D}| \le \alpha_1 \frac{1}{\sqrt{at}}\left(\int_0^\infty e^{\alpha_2 s} e^{-\alpha_3 s^2/at}\,ds\right) t^{1/2} c_1 \operatorname{vol} M + \alpha_4(a+b)t\operatorname{vol} M + dt\operatorname{vol} M t^{n/2}.$$

As $t \downarrow 0$, the right hand side is of order $t^{1/2}$. Moreover, all the constants occurring can be bounded using the geometric properties of M, specified in our hypothesis (i).

In case (ii), a similar argument gives

$$\begin{aligned} &|(4\pi t)^{n/2}\operatorname{Tr} E_{\mathscr{D}}(t) - \operatorname{vol}\mathscr{D}| \\ &\quad \le \alpha_1 \frac{1}{\sqrt{at}}\left(\int_0^\infty e^{\alpha_2 s} e^{-\alpha_3 s^2/at}\right) t^{1/2} c_2 \operatorname{vol} B(p, R+1) \\ &\qquad + \alpha_4(a+b)t\operatorname{vol} B(p, R+1) + dt\operatorname{vol} B(p, R+1)t^{n/2}. \end{aligned}$$

Standard comparison theory [8] gives an upper bound of vol $B(p, R+1)$, employing R and a lower bound for the Ricci curvature of $B(p, R+1)$. It follows that δ exists and has the required geometric dependence.

Our main result on approximating the volume using finitely many eigenvalues is:

THEOREM 4.3. *Let $\varepsilon > 0$ be given. Then for $\delta > 0$ sufficiently small and a positive integer $N(\delta)$ one has*

$$\left|(4\pi\delta)^{n/2}\sum_{i=1}^{N(\delta)} e^{-\lambda_i\delta} - \operatorname{vol}\mathscr{D}\right| < c_4\delta^{1/2} < \varepsilon.$$

Furthermore:

(i) If M is compact, then δ, $N(\delta)$, and c_4 depend upon an upper bound for the volume and sectional curvature of M, a lower bound for the Ricci curvature of M, and a lower bound for the convexity radius of M.

(ii) If M is noncompact, assume $\mathscr{D}$ is contained in a geodesic ball $B(p, R)$. Then $\delta, N(\delta)$ and c_4 depend upon R, an upper bound for the sectional curvatures of $B(p, R + 1)$, a lower bound for the Ricci curvatures of $B(p, R + 1)$, and a lower bound for the convexity radius of $B(p, R + 1)$.

Proof. In [7], it was shown that there exist constants m and c_5 so that $\lambda_i \geq c_5 i^{2/n}$ for all $i \geq m$. Moreover, m and c_5 depend upon the given geometric data. Consequently, if δ is taken from Lemma 4.2, we may choose $N(\delta)$ so that

$$\sum_{i=N(\delta)+1}^{\infty} e^{-\lambda_i \delta} \leq \sum_{i=N(\delta)+1}^{\infty} e^{-c_5 i^{2/n} \delta} < c_6 \delta^{1/2} < \varepsilon/2$$

where c_6 and $N(\delta)$ again have the required geometric dependence.

Applying the triangle inequality,

$$\left| (4\pi\delta)^{n/2} \sum_{i=1}^{N(\delta)} e^{-\lambda_i \delta} - \operatorname{vol} \mathscr{D} \right| \leq c_6 \delta^{1/2} + |(4\pi\delta)^{n/2} \operatorname{Tr} E_{\mathscr{D}}(\delta) - \operatorname{vol} \mathscr{D}|$$

since $\operatorname{Tr} E_{\mathscr{D}}(t) = \sum_{i=1}^{\infty} e^{-\lambda_i t}$. Theorem 4.3 now follows by quoting Lemma 4.2.

If $M = R^n$, and $\mathscr{D}$ is convex, then a lemma of Li and Yau [11] estimates the outradius of $\mathscr{D}$ using a finite part of the spectrum of Δ, acting on $L^2\mathscr{D}$ with Dirichlet boundary conditions. This provides a significant improvement of Theorem 4.3(ii), when M is Euclidean. It would be quite interesting to extend the Li–Yau lemma on more general Riemannian manifolds M.

References

1. N. Angelescu, and G. Nenciu, *On the independence of the thermodynamic limit on the boundary conditions in quantum statistical mechanics*, Comm. Math. Phys., vol. 29 (1973), pp. 15–30.
2. M. van den Berg, *A uniform bound on trace* $(e^{t\Delta})$ *for convex regions in* R^n *with smooth boundaries*, Comm. Math. Phys., vol. 92 (1984), pp. 525–530.
3. Yu D. Burago and V.A. Zalgaller, *Geometric inequalities*, Springer Verlag, N.Y., 1988.
4. J. Cheeger and S.T. Yau, *A lower bound for the heat kernel*, Comm. Pure Appl. Math., vol. 34 (1981), pp. 465–480.
5. J. Dodziuk, *Maximum principle for parabolic inequalities and the heat flow on open manifolds*, Indiana Univ. Math. J., vol. 32 (1983), pp. 703–716.
6. H. Donnelly and P. Li, *Lower bounds for the eigenvalues of negatively curved manifolds*, Math. Z., vol. 172 (1980), pp. 29–40.
7. ______, *Lower bounds for the eigenvalues of Riemannian manifolds*, Michigan Math. J., vol. 29 (1982), pp. 149–161.

8. A. GRAY, *Comparison theorems for the volumes of tubes as generalizations of the Weyl tubes formula*, Topology, vol. 21 (1982), pp. 201–228.
9. V.K. IONIN, *On isoperimetric and various other inequalities for a manifold of bounded curvature*, Siberian Math. J., vol. 10 (1969), pp. 329–342.
10. J. LEE, *Hearing the volume of a drum in hyperbolic space*, Indiana Univ. Math. J., vol. 39 (1990), pp. 585–616.
11. A. TREIBERGS, *Approximating the area of convex domains from a finite part of the spectrum: lecture on a theorem of Li and Yau*, preprint.
12. F. WARNER, *Extension of the Rauch comparison theorem to submanifolds*, Trans. Amer. Math. Soc., vol. 122 (1966), pp. 341–356.

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