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A Uniform Bound on Trace ($e^{t\Delta}$) for Convex Regions in R^n with Smooth Boundaries

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Abstract. We prove a bound (uniform in $t>0$) on trace ($e^{t\Delta}$) for convex domains in R^n with bounded curvature.

1. Introduction

Let D be a bounded domain in R^n with a smooth boundary ∂D. Let $\lambda_1 > \lambda_2 \geqq \lambda_3 \geqq \dots$ be the eigenvalues of the eigenvalue problem

$$\Delta\phi = \lambda\phi \quad \text{on } D, \tag{1}$$

and

$$\phi = 0 \quad \text{on } \partial D. \tag{2}$$

It is well known that

$$Z(t) = \mathrm{trace}(e^{t\Delta}) = \sum_{j=1}^{\infty} e^{t\lambda_j} \tag{3}$$

exists for all $t>0$, and that $Z(t)$ has an asymptotic expansion [1] of the form

$$Z(t) - \frac{1}{(4\pi t)^{n/2}} \cdot \sum_{k=0}^{K} c_k t^{k/2} = O(t^{(K-n+1)/2}), \qquad t \to 0. \tag{4}$$

The coefficients c_0, c_1, and c_2 have been calculated by McKean and Singer [4]. They depend on the geometrical properties of the domain D. For example

$$c_0 = |D| = \text{volume of } D, \tag{5}$$

and

$$c_1 = -\frac{\sqrt{\pi}}{2}|\partial D| = -\frac{\sqrt{\pi}}{2} \cdot \text{surface area of } \partial D. \tag{6}$$

In the special case of a two-dimensional domain ($n=2$) the coefficients $c_0, c_1, \dots, c_6$ are known [2–7].

On the other hand it was shown [8] that for convex domains in R^n there exists a bound on $Z(t)$ which is uniform in t:

$$\left|Z(t)-\frac{|D|}{(4\pi t)^{n/2}}\right| \leqq \frac{e^{n/2}\cdot|\partial D|}{2\cdot(4\pi t)^{(n-1)/2}}, \qquad t>0. \tag{7}$$

Bounds like (7) are useful in quantum statistical mechanics [8, 9]. In this paper we will derive such a uniform bound on $Z(t)$ taking the first two terms of its asymptotic expansion into account. The main result is the following

Theorem. *Let D be a bounded convex domain in R^n $(n=2,3,\ldots)$ with a boundary ∂D such that at each point x of ∂D the curvature is bounded from above by $\frac{1}{R}$ $(R>0)$, then for all t*

$$\left|Z(t)-\frac{|D|}{(4\pi t)^{n/2}}+\frac{|\partial D|}{4\cdot(4\pi t)^{(n-1)/2}}\right| \leqq \frac{|\partial D|\cdot t}{(4\pi t)^{n/2}R}\left\{b_1(n)+b_2(n)\log\left(1+\frac{R^2}{t}\right)\right\}, \tag{8}$$

where

$$b_1(n)=\pi^{1/2}\cdot n(n^{3/2}+\tfrac{1}{2}), \tag{9}$$

and

$$b_2(n)=n-1. \tag{10}$$

We see from (8) that the bound is small compared to the second term in the asymptotic expansion of $Z(t)$ for $\frac{t}{R^2}$ much smaller than one.

2. Pointwise Estimates on the Heat Kernel

In order to prove the theorem we need some pointwise estimates on the heat kernel $K_D(x,y;t)$ corresponding to the operator $\Delta-\frac{\partial}{\partial t}$. By means of the Feynman-Kac formula we see that $K_D(x,y;t)$ is increasing in the domain D. Exploiting this we are able to prove the following lemmas.

Lemma 1. *Let D be a domain in R^n with a smooth boundary ∂D, and let x be a point in D with distance $\partial(x)$ to ∂D. Then*

$$\left|K_D(x,x;t)-\frac{1}{(4\pi t)^{n/2}}\right| \leqq \frac{2n}{(4\pi t)^{n/2}}\exp\left[-\frac{\partial^2(x)}{nt}\right], \qquad t>0. \tag{11}$$

For the proof we refer to [10].

Lemma 2. *Let D be a convex domain in R^n, then for x in D*

$$K_D(x,x;t) \leqq \frac{1}{(4\pi t)^{n/2}}\left(1-\exp\left[-\frac{\partial^2(x)}{t}\right]\right), \qquad t>0. \tag{12}$$

This inequality appears in Kac's paper [3].

Lemma 3. *Let D be a convex domain in R^n with a boundary ∂D such that at each point of ∂D the curvature is bounded from above by $\frac{1}{R}$ $(R>0)$, then for all $x \in D$ such that $\varepsilon \leqq \partial(x) \leqq R$*

$$K_D(x,x;t) \geqq \frac{1}{(4\pi t)^{(n-1)/2}}\left(1-2(n-1)\exp\left[-\frac{\varepsilon R}{t(n-1)}\right]\right) \cdot \frac{1}{R-\varepsilon}\sum_{k=1}^{\infty}\exp\left[-\frac{t\pi^2k^2}{4(R-\varepsilon)^2}\right]\left(\sin\frac{\pi k}{2}\cdot\frac{\partial(x)-\varepsilon}{R-\varepsilon}\right)^2. \tag{13}$$

Proof. For all $x \in D$ such that $\varepsilon < \partial(x) < R$ we can find a cylinder C in R^n with radius $(\varepsilon R)^{1/2}$ and an axis A_C with length $2(R-\varepsilon)$ such that:

1. $x \in C$,
2. $C \subset D$,
3. $x \in A_C$ and x has a distance $\partial(x)-\varepsilon$ to the endpoint of the axis.

By the monotonicity of $K_D(x,x;t)$ we obtain

$$K_D(x,x;t) \geqq K_{\odot}(0,0;t)\cdot\frac{1}{R-\varepsilon}\sum_{k=1}^{\infty}\exp\left[-\frac{t\pi^2k^2}{4(R-\varepsilon)^2}\right]\left(\sin\frac{\pi k}{2}\cdot\frac{\partial(x)-\varepsilon}{R-\varepsilon}\right)^2, \tag{14}$$

where $K_{\odot}(0,0;t)$ is the heat kernel corresponding to $\Delta-\frac{\partial}{\partial t}$ with zero boundary conditions on a $(n-1)$-dimensional sphere $\odot$ with radius $(\varepsilon R)^{1/2}$, evaluated at the centre of $\odot$.

By Lemma 1 we find

$$K_{\odot}(0,0;t) \geqq \frac{1}{(4\pi t)^{(n-1)/2}}\left(1-2(n-1)\exp\left[-\frac{\varepsilon R}{t(n-1)}\right]\right), \tag{15}$$

which proves Lemma 3. □

If we write $K_D(x,y;t)$ in its eigenfunction expansion

$$K_D(x,y;t)=\sum_{j=1}^{\infty} e^{t\lambda_j}\phi_j(x)\phi_j(y) \tag{16}$$

[where $\phi_1(x)$, $\phi_2(x)$, $\phi_3(x)$, ... is the orthonormal set of eigenfunctions of the problem (1), (2)], we see that

$$Z(t)=\int_{x\in D} K_D(x,x;t)\cdot dx. \tag{17}$$

3. The Proof

In order to prove the theorem we will make extensive use of Steiner's theorem (4.3 of [11]) which we will state here in a modified form.

Theorem (Steiner). *Let D be a convex domain in R^n with volume $|D|$, a boundary ∂D with surface area $|\partial D|$ and at each point of ∂D a curvature bounded above by $\frac{1}{R}$ $(R>0)$. Let D_y be a family of regions contained in D with a surface δD_y parallel* *to ∂D at distance y, then*

$$|D_x| = |D| - \int_0^x |\partial D_y| dy, \qquad 0 \leqq x \leqq R, \tag{18}$$

$$|\partial D_x| \geqq |\partial D| \cdot \left(1 - \frac{(n-1)x}{R}\right), \tag{19}$$

$$|D_x| \leqq |D_y|, \qquad |\partial D_x| \leqq |\partial D_y|, \qquad x \geqq y, \tag{20}$$

and the curvature at each point of D_y is bounded above by $(R-y)^{-1}$ for all $0 \leqq y < R$.

Proof of Theorem. If we integrate (11) with respect to x over D we get

$$\left| Z(t) - \frac{|D|}{(4\pi t)^{n/2}} \right| \leqq \frac{n^{3/2} \cdot |\partial D|}{2 \cdot (4\pi t)^{(n-1)/2}}. \tag{21}$$

Notice that (21) is a sharper bound than (7) for $n = 3, 4, \ldots$. From (21) it follows that

$$\left| Z(t) - \frac{|D|}{(4\pi t)^{n/2}} + \frac{|\partial D|}{4 \cdot (4\pi t)^{(n-1)/2}} \right| \leqq \frac{|\partial D| \cdot t}{(4\pi t)^{n/2} \cdot R} \cdot \pi^{1/2} \cdot n \left(n^{3/2} + \frac{1}{2} \right), \tag{22}$$

for all $t \geqq \frac{R^2}{n^2}$.

By Lemma 2, (18) and (19) we obtain an upper bound on $Z(t)$:

$$\begin{aligned} Z(t) &\leqq \frac{|D|}{(4\pi t)^{n/2}} - \frac{1}{(4\pi t)^{n/2}} \int_{\{x \in D : 0 \leqq \partial(x) \leqq R\}} \exp\left[-\frac{\partial^2(x)}{t} \right] dx \\ &= \frac{|D|}{(4\pi t)^{n/2}} - \frac{1}{(4\pi t)^{n/2}} \int_0^R \exp\left(-\frac{y^2}{t} \right) |\partial D_y| dy \\ &\leqq \frac{|D|}{(4\pi t)^{n/2}} - \frac{|\partial D|}{4 \cdot (4\pi t)^{(n-1)/2}} + \frac{|\partial D|}{(4\pi t)^{n/2}} \left\{ \int_R^\infty \exp\left(-\frac{y^2}{t} \right) dy + \frac{n-1}{R} \int_0^R \exp\left(-\frac{y^2}{t} \right) y dy \right\} \\ &\leqq \frac{|D|}{(4\pi t)^{n/2}} - \frac{|\partial D|}{4 \cdot (4\pi t)^{(n-1)/2}} + \frac{(n-1)|\partial D| \cdot t}{(4\pi t)^{n/2} \cdot 2R}. \end{aligned} \tag{23}$$

Let

$$A(t) \equiv \int_{\{x \in D : \varepsilon \leqq \partial(x) \leqq R\}} K_D(x, x; t) dx, \tag{24}$$

and

$$B(t) \equiv \int_{\{x \in D : \partial(x) \geqq R\}} K_D(x, x; t) dx, \tag{25}$$

so that $Z(t) \geqq A(t) + B(t)$. We use Lemma 1 to obtain a lower bound on $B(t)$:

$$\begin{aligned} B(t) &\geqq \frac{1}{(4\pi t)^{n/2}} \left\{ |D_R| - 2n |\partial D| \int_R^\infty \exp\left(-\frac{y^2}{nt} \right) dy \right\} \\ &\geqq \frac{1}{(4\pi t)^{n/2}} \left\{ |D_R| - n^2 |\partial D| \cdot \frac{t}{R} \right\}. \end{aligned} \tag{26}$$

For $A(t)$ we find

$$A(t) \geqq \int_{\varepsilon}^{R} |\partial D| \cdot K_{\odot}(0,0;t) \cdot \frac{1}{R-\varepsilon} \sum_{k=1}^{\infty} \exp\left[-\frac{t\pi^2 k^2}{4(R-\varepsilon)^2}\right]\left(\sin\frac{\pi k}{2}\cdot\frac{y-\varepsilon}{R-\varepsilon}\right)^2 dy$$
$$-\int_{\varepsilon}^{R} (|\partial D| - |\partial D_y|)\frac{1}{(4\pi t)^{n/2}} \cdot dy. \tag{27}$$

The second term in (27) is bounded from below by

$$-\frac{1}{(4\pi t)^{n/2}}(|\partial D| \cdot R - |D| + |D_R|), \tag{28}$$

since $|\partial D_x| \leqq |\partial D|$.

The first term in (27) is bounded from below by

$$\frac{1}{(4\pi t)^{(n-1)/2}}\left(1-2(n-1)\exp\left[-\frac{\varepsilon R}{t(n-1)}\right]\right)\cdot\frac{|\partial D|}{2}\cdot\sum_{k=1}^{\infty}\exp\left[-\frac{t\pi^2k^2}{4(R-\varepsilon)^2}\right]$$
$$\geqq \frac{1}{(4\pi t)^{(n-1)/2}}\left(1-2(n-1)\exp\left[-\frac{\varepsilon R}{t(n-1)}\right]\right)\cdot\frac{|\partial D|}{2}\cdot\left(\frac{R-\varepsilon}{(\pi t)^{1/2}}-\frac{1}{2}\right) \tag{29}$$

for all $\varepsilon \leqq R$ and

$$\exp\left[-\frac{\varepsilon R}{t(n-1)}\right] < \frac{1}{2(n-1)}. \tag{30}$$

Combining (26), (28), and (29) we have

$$Z(t) \geqq \frac{D}{(4\pi t)^{n/2}} - \frac{|\partial D|}{4\cdot(4\pi t)^{(n-1)/2}} - \frac{|\partial D|}{(4\pi t)^{n/2}}\left\{\frac{n^2 t}{R} + \varepsilon + 2(n-1)R\exp\left[-\frac{\varepsilon R}{t(n-1)}\right]\right\}, \tag{31}$$

subject to (30). Choose

$$\varepsilon = \frac{t(n-1)}{R}\cdot\log\left(\frac{2R^2}{t}\right), \quad \text{for} \quad t \leqq \frac{R^2}{n^2}. \tag{32}$$

Combining (31)–(33) we get for $t \leqq \dfrac{R^2}{n^2}$:

$$\left|Z(t) - \frac{|D|}{(4\pi t)^{n/2}} + \frac{|\partial D|}{4\cdot(4\pi t)^{(n-1)/2}}\right| \leqq \frac{|\partial D|\cdot t}{(4\pi t)^{n/2}\cdot R}\left\{\frac{3}{2}(n-1) + n^2 + (n-1)\log\left(\frac{2R^2}{t}\right)\right\}. \tag{33}$$

But $\log\dfrac{R^2}{t} < \log\left(1+\dfrac{R^2}{t}\right)$ for all $t>0$, and the theorem follows since

$$n^2 + (n-1)(\tfrac{3}{2} + \log 2) \leqq \pi^{1/2} n (n^{3/2} + \tfrac{1}{2}), \qquad n = 2, 3, \ldots. \quad \square$$

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