Analysis of the heat equation on Riemannian manifolds

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1 Introduction: Laplace-Beltrami operator and heat kernel

Let (M,g) be a connected Riemannian manifold. The Laplace-Beltrami operator Δ is given in the local coordinates by

$$\Delta = \frac{1}{\sqrt{\det g}} \sum_{i,j=1}^{n} \frac{\partial}{\partial x^i}\left(\sqrt{\det g} g^{ij} \frac{\partial}{\partial x^j}\right),$$

where $n = \dim M$, $g = (g_{ij})$ and $(g^{ij}) = g^{-1}$. This operator is symmetric with respect to the Riemannian measure

$$d\mu = \sqrt{\det g} dx^1 ... dx^n,$$

that is, for all $u, v \in C_0^\infty(M)$,

$$\int_M (\Delta u)\, v\, d\mu = -\int_M \langle \nabla u, \nabla v\rangle\, d\mu = \int_M u \Delta v\, d\mu$$

Furthermore, the operator Δ with the domain $C_0^\infty(M)$ is admits the Friedrichs extension to a self-adjoint operator in $L^2(M,\mu)$ that will also be denoted by Δ. This operator is non-positive definite since for all $u \in C_0^\infty$

$$(\Delta u, u)_{L^2} = \int_M (\Delta u)\, u\, d\mu = -\int_M |\nabla u|^2\, d\mu \le 0.$$

Hence, $\operatorname{spec}\Delta \subset (-\infty, 0]$.

The *heat semigroup* of M is a family $\{P_t\}_{t\ge 0}$ of self-adjoint operators defined by

$$P_t = \exp(t\Delta)$$

using the functional calculus of self-adjoint operators. Since the function $\lambda \mapsto \exp(t\lambda)$ is bounded for $\lambda \in (-\infty, 0]$, that is, on the spectrum of Δ, it follows that P_t is a bounded self-adjoint operator in $L^2(M,\mu)$.

For any $f \in L^2(M,\mu)$, the function

$$u(t,x) = P_t f(x)$$

is a smooth function of $(t,x) \in \mathbb{R}_+ \times M$, satisfies the heat equation $\frac{\partial u}{\partial t} = \Delta u$ and the initial condition

$$u(t,\cdot) \overset{L^2}{\to} f \quad \text{as } t \to 0+.$$

The *heat kernel* $p_t(x,y)$ is a function of $t > 0$ and $x, y \in M$ such that

$$P_t f(x) = \int_M p_t(x,y) f(y)\, d\mu(y),$$

for all $f \in L^2(M,\mu)$. It is known that $p_t(x,y)$ exists on any Riemannian manifold and is unique. Besides, the heat kernel satisfies the following properties.

- Smoothness: $p_t(x,y) \in C^\infty(\mathbb{R}_+ \times M \times M)$

- Positivity: $p_t(x,y) > 0$
- Symmetry: $p_t(x,y) = p_t(y,x)$;
- The semigroup identity:

$$p_{t+s}(x,y) = \int_M p_t(x,z)\, p_s(z,y)\, d\mu(z). \tag{1}$$

- Submarkovian property:

$$\int_M p_t(x,y)\, d\mu(y) \le 1.$$

- For any $y \in M$, the function $u(t,x) = p_t(x,y)$ satisfies the heat equation and the initial condition

$$u(t,x) \to \delta_y(x) \quad \text{as } t \to 0+,$$

  that is, $p_t(x,y)$ is a fundamental solution of the heat equation. Moreover, $p_t(x,y)$ is the smallest positive fundamental solution of the heat equation.

Recall that in $\mathbb{R}^n$, Δ is the classical Laplace operator $\Delta = \sum_{k=1}^n \frac{\partial^2}{\partial x_k^2}$, and its heat kernel is given by the Gauss-Weierstrass formula

$$p_t(x,y) = \frac{1}{(4\pi t)^{n/2}} \exp\left(-\frac{|x-y|^2}{4t}\right).$$

Explicit formulas for the heat kernel exist also in hyperbolic spaces $\mathbb{H}^n$. For example in $\mathbb{H}^3$

$$p_t(x,y) = \frac{1}{(4\pi t)^{3/2}} \frac{r}{\sinh r} \exp\left(-\frac{r^2}{4t} - t\right), \tag{2}$$

where $r = d(x,y)$ is the geodesic distance between x, y. For arbitrary $\mathbb{H}^n$ the formula looks complicated, but it implies the following estimate, for all $t > 0$ and $x, y \in \mathbb{H}^n$:

$$p_t(x,y) \simeq \frac{(1+r+t)^{\frac{n-3}{2}}(1+r)}{t^{n/2}} \exp\left(-\lambda t - \frac{r^2}{4t} - \sqrt{\lambda} r\right), \tag{3}$$

where $\lambda = \frac{(n-1)^2}{4}$ is the bottom of the spectrum of the Laplace operator on $\mathbb{H}^n$.

2 Faber-Krahn inequality

Any open set $\Omega \subset M$ can be regarded as a Riemannian manifold, too. Hence, the Laplace operator Δ initially defined on $C_0^\infty(\Omega)$ admits the Friedrichs extension to a self-adjoint operator in $L^2(\Omega,\mu)$ that will be denoted by Δ_Ω and that is non-positive definite. It is called the *Dirichlet Laplacian* in Ω. Set

$$\lambda_{\min}(\Omega) = \inf \operatorname{spec}(-\Delta_\Omega).$$

By the variational property we have

$$\begin{aligned}\lambda_{\min}(\Omega) &= \inf_{f\in \mathrm{dom}(\Delta_\Omega)\setminus\{0\}} \frac{(-\Delta_\Omega f, f)}{\|f\|_{L^2}^2} \\ &= \inf_{f\in C_0^\infty(\Omega)\setminus 0} \frac{(-\Delta_\Omega f, f)}{\|f\|_{L^2}^2} \\ &= \inf_{f\in C_0^\infty(\Omega)\setminus 0} \frac{\int_\Omega |\nabla f|^2 \, d\mu}{\|f\|_{L^2}^2} \\ &= \inf_{f\in \mathrm{Lip}_0(\Omega)\setminus 0} \frac{\int_\Omega |\nabla f|^2 \, d\mu}{\|f\|_{L^2}^2}.\end{aligned}$$

The quantity

$$\frac{\int_\Omega |\nabla f|^2 \, d\mu}{\|f\|_{L^2}^2}$$

is called the *Rayleigh quotient* of f in Ω.

Definition. We say that Ω satisfies the Faber-Krahn inequality if, for any non-empty open set $U \Subset \Omega$ we have

$$\lambda_{\min}(U) \geq a\mu(U)^{-\beta}, \tag{4}$$

for some $a, \beta > 0$.

The exponent β is usually equal to $2/n$ where $n = \dim M$. The parameter a is called the Faber-Krahn constant of Ω. It depends on the intrinsic geometry of Ω.

Let $\Omega = \mathbb{R}^n$. By the *Faber-Krahn theorem*, for any precompact open domain $U \subset \mathbb{R}^n$, we have

$$\lambda_{\min}(U) \geq \lambda_{\min}(U^*),$$

where U^* is a ball of the same volume as U. If the radius of U^* is r then

$$\lambda_{\min}(U^*) = \frac{c_n}{r^2}$$

with some positive constant c_n. Since

$$\mu(U) = \mu(U^*) = b_n r^n,$$

it follows that

$$\lambda_{\min}(U) \geq a_n \mu(U)^{-2/n}, \tag{5}$$

where $a_n > 0$. Hence, $\mathbb{R}^n$ satisfies the Faber-Krahn inequality (4) with $a = a_n$ and $\beta = 2/n$.

Using this fact, it is easy to prove, using the compactness argument that any relatively compact open set $\Omega \subset M$ on any Riemannian manifold M also satisfies the Faber-Krahn inequality (4) with some $a = a(\Omega) > 0$ and $\beta = 2/n$, where $n = \dim M$.

It is possible to prove the following two facts.

1. If M is a Cartan-Hadamard manifold (that is, a simply connected manifold of non-positive sectional curvature) then M satisfies the Faber-Krahn inequality (4) with some $a > 0$ and $\beta = 2/n$ (and, hence, any open domain $\Omega \subset M$ also satisfies the same inequality).

2. If M is complete manifold of non-negative Ricci curvature then any geodesic ball $B = B(x, R)$ in M satisfies the Faber-Krahn inequality (5) with the Faber-Krahn constant

$$a = a(B) = c\frac{\mu(B)^{2/n}}{R^2} \tag{6}$$

and $\beta = 2/n$ where $c = c(n) > 0$.

In particular, if in addition

$$\mu(B) \simeq R^n$$

(as in $\mathbb{R}^n$) then it follows that $a(B)$ may be chosen to be independent of balls so that also the entire manifold M has also the same Faber-Krahn constant.

Another example. Let $M = K \times \mathbb{R}^m$ where K is a compact manifold of dimension $n-m$. Any ball $B = B(x, R)$ on this manifold has the Faber-Krahn constant (6). Since

$$\mu(B) \simeq \begin{cases} R^n, & R < 1 \\ R^m, & R \geq 1, \end{cases}$$

we obtain that

$$a(B) \simeq \begin{cases} 1, & R < 1 \\ R^{2m/n-2}, & R \geq 1 \end{cases}$$

Proposition 1 *Suppose that for any domain $U \Subset \Omega$ with smooth boundary,*

$$\operatorname{area}(\partial U) \geq b\mu(U)^\gamma$$

for some $b > 0$ and $0 < \gamma < 1$. Then Ω satisfies the Faber-Krahn inequality (4) with $a = \frac{b^2}{4}$ and $\beta = 2(1-\gamma)$.

In particular, if $\gamma = \frac{n-1}{n}$ as in $\mathbb{R}^n$ then $\beta = 2/n$.

Proof. For any open domain $U \subset M$ define the Cheeger constant

$$h(U) = \inf_{V \Subset U} \frac{\operatorname{area}(\partial V)}{\mu(V)},$$

where V is any open set with smooth boundary. Since

$$\operatorname{area}(\partial V) \geq b\mu(V)^\gamma,$$

and $\gamma \leq 1$it follows that

$$\frac{\operatorname{area}(\partial V)}{\mu(V)} \geq b\mu(V)^{\gamma-1} \geq b\mu(U)^{\gamma-1}.$$

It follows that

$$h(U) \geq b\mu(U)^{\gamma-1}.$$

By the Cheeger inequality,

$$\begin{aligned} \lambda_{\min}(U) &\geq \frac{1}{4}h(U)^2 \\ &\geq \frac{b^2}{4}\mu(U)^{-2(1-\gamma)}, \end{aligned}$$

which was to be proved. ∎

3 Mean-value inequality

Let I be an interval in $\mathbb{R}$ and Ω be an open subset of $M/$ A C^2 function $u(t,x)$ defined in $I \times \Omega$ is called a subsolution of the heat equation if

$$\partial_t u \leq \Delta u \ \text{ in } I \times \Omega. \tag{7}$$

Theorem 2 (Mean value inequality) *Let $B(x,R)$ be a relatively compact ball in M that satisfies the Faber-Krahn inequality (4). Let $u(t,y)$ be a non-negative subsolution of the heat equation in $(0,T] \times B(x,R)$ for some $T > 0$. Then we have*

$$u^2(T,x) \leq \frac{Ca^{-1/\beta}}{\min(T,R^2)^{1+1/\beta}} \int_0^T \int_{B(x,R)} u^2(t,y)\, d\mu(y) dt, \tag{8}$$

where $C = C(\beta)$.

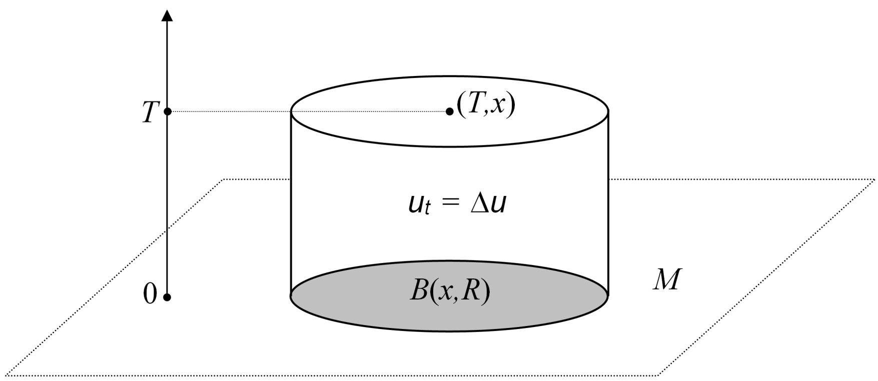


Illustration to mean-value inequality

In particular, if $\beta = 2/n$ then (8) becomes

$$u^2(T,x) \leq \frac{Ca^{-n/2}}{\min(T,R^2)^{1+n/2}} \int_0^T \int_{B(x,R)} u^2(t,y)\, d\mu(y) dt,$$

Define measure ν on $\mathbb{R} \times M$ by

$$d\nu = d\mu dt$$

and prove first two lemmas.

Lemma 3 *Let Ω be an open subset of M and $T > 0$. Let $\eta(t,x)$ be a Lipschitz function in the cylinder*

$$\mathcal{C} = [0,T] \times \Omega$$

such that $\operatorname{supp} \eta \subset [0,T] \times K$ for some compact set $K \subset \Omega$. Let u be a subsolution to the heat equation in $\mathcal{C}$ and set $v = (u - \theta)_+$ with some real θ. Then the following inequality holds:

$$\frac{1}{2}\left[\int_\Omega v^2\eta^2(t,\cdot)\, d\mu\right]_{t=0}^{T} + \int_{\mathcal{C}} |\nabla(v\eta)|^2 d\nu \leq \int_{\mathcal{C}} v^2 \left(|\nabla\eta|^2 + \eta\partial_t\eta\right) d\nu. \tag{9}$$

In particular, if $\eta(0,\cdot)=0$ *then*

$$\int_{\mathcal{C}} |\nabla(v\eta)|^2 \, d\nu \le \int_{\mathcal{C}} v^2 \left(|\nabla\eta|^2 + \eta\partial_t\eta\right) d\nu \tag{10}$$

and, for any $t\in[0,T]$,

$$\int_{\Omega} v^2\eta^2(t,\cdot)\,d\mu \le 2\int_{\mathcal{C}} v^2\left(|\nabla\eta|^2+\eta\partial_t\eta\right)d\nu. \tag{11}$$

Proof. The estimate (10) is an obvious consequence of (9). The estimate (11) follows from (9) if one replaces T by t.

Let us prove (9). The function $v(t,\cdot)$ is locally Lipschitz. For the weak gradient of v we have

$$\nabla v = 1_{\{u>\theta\}}\nabla u = 1_{\{v\neq 0\}}\nabla u,$$

which implies

$$\langle\nabla u,\nabla v\rangle = |\nabla v|^2 \quad\text{and}\quad v\nabla u = v\nabla v. \tag{12}$$

Since $\eta(t,\cdot)\in \mathrm{Lip}_0(\Omega)$, we have also $v\eta^2\in\mathrm{Lip}_0(\Omega)$ for any fixed time t and

$$\nabla\left(v\eta^2\right) = v\nabla\eta^2+\eta^2\nabla v = 2v\eta\nabla\eta+\eta^2\nabla v,$$

whence

$$\langle\nabla u,\nabla\left(v\eta^2\right)\rangle = 2v\eta\langle\nabla v,\nabla\eta\rangle+\eta^2|\nabla v|^2.$$

Multiplying the inequality (7) by $v\eta^2$ and integrating over $\mathcal{C}$, we obtain

$$\begin{aligned}
\int_{\mathcal{C}}\partial_t u\, v\eta^2 d\nu &\le \int_0^T\int_{\Omega}(\Delta u)\,v\eta^2 d\mu dt\\
&= -\int_0^T\int_{\Omega}\langle\nabla u,\nabla\left(v\eta^2\right)\rangle d\mu dt\\
&= -\int_{\mathcal{C}}\left(2v\eta\langle\nabla u,\nabla\eta\rangle+\eta^2\langle\nabla u,\nabla v\rangle\right)d\nu\\
&= -\int_{\mathcal{C}}\left(2v\eta\langle\nabla v,\nabla\eta\rangle+\eta^2|\nabla v|^2\right)d\nu,
\end{aligned}$$

where we have used the Green formula and (12).

Since

$$|\nabla(v\eta)|^2 = (\eta\nabla v+v\nabla\eta)^2 = \eta^2|\nabla v|^2+v^2|\nabla\eta|^2+2v\eta\langle\nabla v,\nabla\eta\rangle,$$

we have

$$2v\eta\langle\nabla v,\nabla\eta\rangle+\eta^2|\nabla v|^2 = |\nabla(v\eta)|^2-v^2|\nabla\eta|^2,$$

whence it follows that

$$\int_{\mathcal{C}}\partial_t u\,v\eta^2 d\nu \le -\int_{\mathcal{C}}|\nabla(v\eta)|^2 d\nu+\int_{\mathcal{C}}v^2|\nabla\eta|^2 d\nu. \tag{13}$$

For any fixed x, all functions u, v, η are Lipschitz in $t \in [0, T]$. Therefore, using the integration by parts formula for Lipschitz functions of t, we obtain, for any fixed $x \in \Omega$,

$$\begin{aligned}\int_0^T \partial_t u\, v\eta^2 dt &= \frac{1}{2}\int_0^T \partial_t\left(v^2\right)\eta^2 dt \\ &= \frac{1}{2}\left[v^2\eta^2\right]_0^T - \frac{1}{2}\int_0^T v^2\partial_t\left(\eta^2\right)dt = \frac{1}{2}\left[v^2\eta^2\right]_0^T - \int_0^T v^2\eta\partial_t\eta dt.\end{aligned}$$

Integrating this identity over Ω, we obtain

$$\int_{\mathcal{C}} \partial_t u\, v\eta^2 d\nu = \frac{1}{2}\left[\int_\Omega v^2\eta^2 d\mu\right]_0^T - \int_{\mathcal{C}} v^2\eta\partial_t\eta\, d\nu$$

and combining with (13)

$$\frac{1}{2}\left[\int_\Omega v^2\eta^2 d\mu\right]_0^T - \int_{\mathcal{C}} v^2\eta\partial_t\eta\, d\nu \le -\int_{\mathcal{C}}\left|\nabla\left(v\eta\right)\right|^2 d\nu + \int_{\mathcal{C}} v^2\left|\nabla\eta\right|^2 d\nu,$$

which is equivalent to (9). ■

Lemma 4 *Let $B(x,R)$ be a relatively compact ball in M that satisfies the Faber-Krahn inequality (4). Let $u(t,y)$ be a subsolution of the heat equation in $\mathcal{C} = (0,T] \times B(x,R)$ for some $T > 0$. Consider two smaller cylinders*

$$\mathcal{C}_k = [T_k, T] \times B(x, R_k),\ k = 0, 1,$$

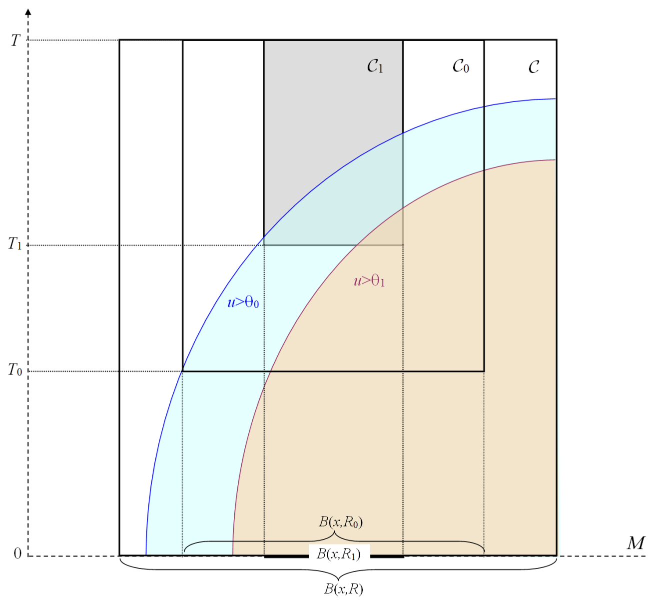
where $0 < R_1 < R_0 \le R$ and $0 \le T_0 < T_1 < T$. Choose $\theta_1 > \theta_0$ and set

$$J_k = \int_{\mathcal{C}_k} (u - \theta_k)_+^2\, d\nu.$$

Then the following inequality holds

$$J_1 \le \frac{C J_0^{1+\beta}}{a\delta^{1+\beta}\left(\theta_1 - \theta_0\right)^{2\beta}}, \tag{14}$$

where $C = C(\beta)$ and $\delta = \min\left(T_1 - T_0, (R_0 - R_1)^2\right)$.



Cylinders $\mathcal{C}$, $\mathcal{C}_0$ and $\mathcal{C}_1$

Proof. Replacing function u by $u-\theta_0$ we can assume that $\theta_0=0$ and rename θ_1 to θ so that $\theta>0$. Without loss of generality and to simplify notation we can assume that $T_0=0$. Set for any $\lambda\in[0,1]$

$$R_\lambda=\lambda R_1+(1-\lambda)\,R_0.$$

Consider a function

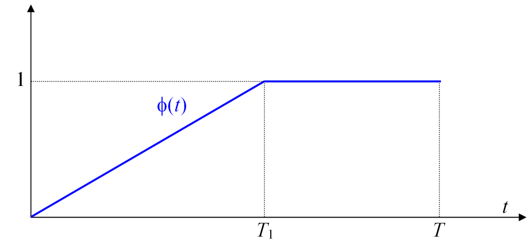
$$\eta(t,y)=\varphi(t)\,\psi(y)\,,$$

where

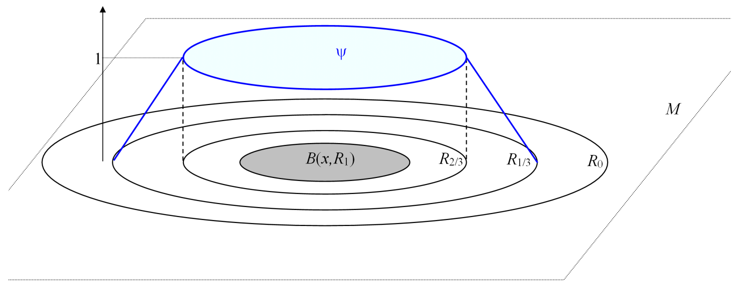
$$\varphi(t)=\frac{t}{T_1}\wedge 1 \tag{15}$$

and

$$\psi(y)=\frac{\left(R_{1/3}-d(x,y)\right)_+}{R_{1/3}-R_{2/3}}\wedge 1. \tag{16}$$



Function $\phi(t)$ given by (15)



Function ψ given by (16)

Obviously,

$$\psi=1\ \text{ on }\ B\left(x,R_{2/3}\right)\quad\text{ and }\quad\operatorname{supp}\psi=\overline{B\left(x,R_{1/3}\right)}.$$

Applying the estimate (11) of Lemma 3 in the cylinder $\mathcal{C}_0=[0,T]\times B(x,R_0)$ for function $v=u_+$ with $t\in[T_1,T]$ and noticing that $\eta(t,y)=1$ for t in this range and $y\in B\left(x,R_{2/3}\right)$, we obtain

$$\int_{B\left(x,R_{2/3}\right)}u_+^2(t,\cdot)\,d\mu\leq\int_{B(x,R_0)}u_+^2\eta^2(t,\cdot)\,d\mu\leq 2\int_{\mathcal{C}_0}u_+^2\left(|\nabla\eta|^2+\eta\partial_t\eta\right)d\nu\leq\frac{20}{\delta}J_0, \tag{17}$$

where we have also used that

$$|\nabla\eta|^2\leq\frac{1}{\left(R_{1/3}-R_{2/3}\right)^2}=\frac{9}{\left(R_0-R_1\right)^2}\leq\frac{9}{\delta}$$

and

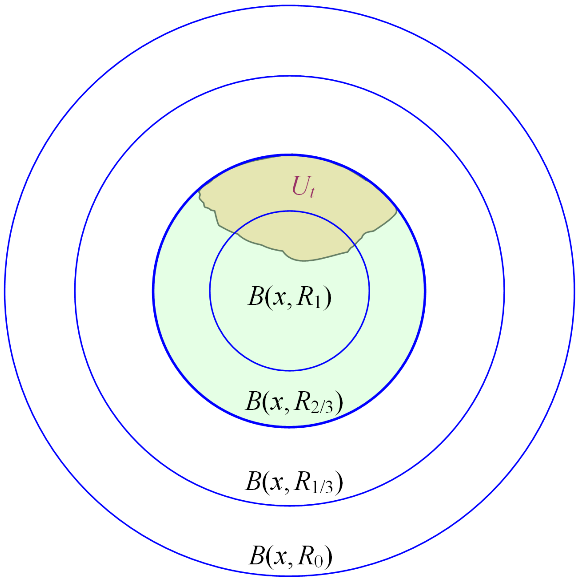
$$\eta\partial_t\eta\leq\frac{1}{T_1}\leq\frac{1}{\delta}.$$

For any $t\in[T_1,T]$, consider the set

$$U_t=\left\{y\in B\left(x,R_{2/3}\right):u(t,y)>\theta\right\}. \tag{18}$$

It follows from (17) that

$$\mu\left(U_t\right) \leq \frac{1}{\theta^2}\int_{B\left(x,R_{2/3}\right)} u_+^2\left(t,\cdot\right)d\mu \leq \frac{20J_0}{\theta^2\delta}. \tag{19}$$



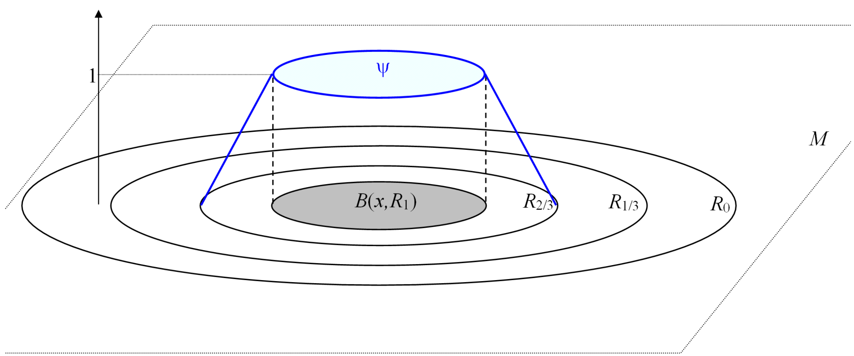
Set U_t defined by (18)

Consider now a different function ψ:

$$\psi\left(y\right) = \frac{\left(R_{2/3} - d\left(x,y\right)\right)_+}{R_{2/3} - R_1} \wedge 1, \tag{20}$$

so that

$$\psi = 1 \quad \text{on} \quad B\left(x,R_1\right) \qquad \text{and} \qquad \operatorname{supp}\psi = \overline{B\left(x,R_{2/3}\right)}.$$



Function ψ given by (20)

Applying (10) for function $v=(u-\theta)_+$ with $\eta(t,x)=\varphi(t)\psi(y)$ where φ is given by (15) and ψ is given by (20), we obtain

$$\int_{\mathcal{C}_0}|\nabla(v\eta)|^2\,d\nu\leq\int_{\mathcal{C}_0}v^2\left(|\nabla\eta|^2+\eta\partial_t\eta\right)d\nu\leq\frac{10}{\delta}\int_{\mathcal{C}_0}v^2d\nu\leq\frac{10}{\delta}J_0. \tag{21}$$

Fix some $t\in[T_1,T]$. The function $(v\eta)(t,y)$ can take a non-zero value only if $y\in B\left(x,R_{2/3}\right)$ and $u(t,y)>\theta$, that is, if $y\in U_t$. It follows that

$$\begin{aligned}\int_{B(x,R_0)}|\nabla(v\eta)|^2(t,\cdot)\,d\mu &\geq \int_{U_t}|\nabla(v\eta)|^2(t,\cdot)\,d\mu\\ &\geq \lambda_{\min}(U_t)\int_{U_t}(v\eta)^2(t,\cdot)\,d\mu\\ &\geq a\mu(U_t)^{-\beta}\int_{B(x,R_0)}(v\eta)^2(t,\cdot)\,d\mu\\ &\geq a\left(\frac{\theta^2\delta}{20}\right)^{\beta}J_0^{-\beta}\int_{B(x,R_1)}v^2(t,\cdot)\,d\mu\end{aligned}$$

where we have used the variational property of $\lambda_{\min}$, the Faber-Krahn inequality, the estimate (19), and that $\eta=1$ in $[T_1,T]\times B(x,R_1)$.

Integrating this inequality in t from T_1 to T and using (21), we obtain

$$\begin{aligned}\frac{10}{\delta}J_0 &\geq \int_{T_1}^{T}\int_{B(x,R_0)}|\nabla(v\eta)|^2\,d\nu\\ &\geq a\left(\frac{\theta^2\delta}{20}\right)^{\beta}J_0^{-\beta}\int_{T_1}^{T}\int_{B(x,R_1)}v^2d\mu dt\\ &= a\left(\frac{\theta^2\delta}{20}\right)^{\beta}J_0^{-\beta}J_1.\end{aligned}$$

It follows that

$$J_1\leq 10\frac{20^\beta}{a\delta^{1+\beta}\theta^{2\beta}}J_0^{1+\beta},$$

which was to be proved. ■

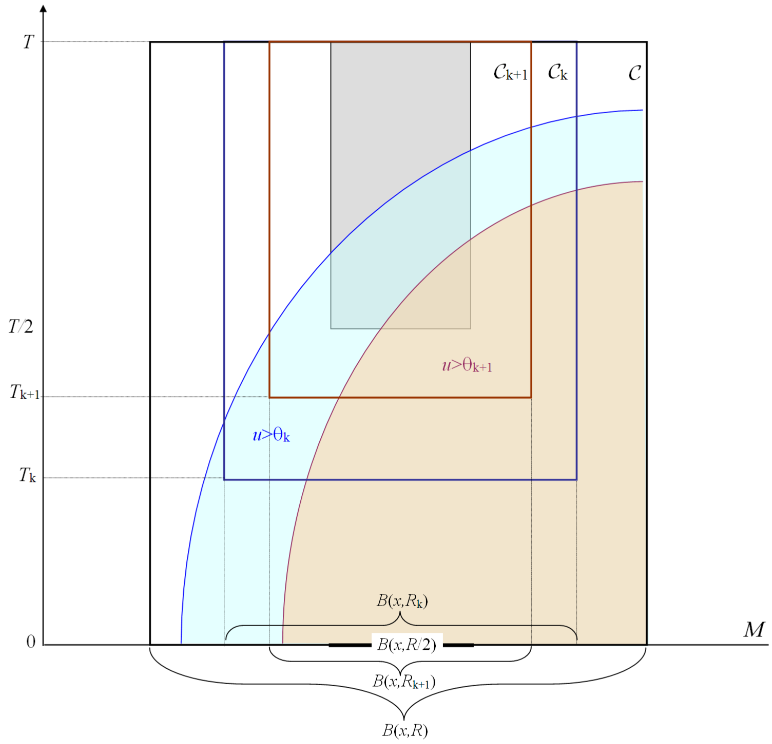
Proof of Theorem 2. Consider a sequence of cylinders

$$\mathcal{C}_k=[T_k,T]\times B(x,R_k),$$

where $\{T_k\}_{k=0}^\infty$ is a strictly increasing sequence such that $T_0=0$ and $T_k\leq T/2$ for all k, and $\{R_k\}_{k=0}^\infty$ is a strictly decreasing sequence such that $R_0=R$ and $R_k\geq R/2$ for all k. Assume also that

$$(R_k-R_{k+1})^2=T_{k+1}-T_k=:\delta_k. \tag{22}$$

In particular, the sequence of cylinders $\{\mathcal{C}_k\}_{k=0}^\infty$ is nested, $\mathcal{C}_0=\mathcal{C}$ and all $\mathcal{C}_k$ contain $[T/2,T]\times B(x,R/2)$ for all k. The values of R_k and T_k will be specified below.



Cylinders $\mathcal{C}_k$

Fix some $\theta > 0$ and set

$$\theta_k = \left(1 - 2^{-(k+1)}\right)\theta$$

so that $\theta_0 = \theta/2$ and $\theta_k \nearrow \theta$ as $k \to \infty$. Set also

$$J_k = \int_{\mathcal{C}_k} (u - \theta_k)^2 \, d\nu.$$

Clearly, the sequence $\{J_k\}_{k=0}^{\infty}$ is decreasing. We will find θ such that $J_k \to 0$ as $k \to \infty$, which will implies that

$$\int_{T/2}^{T} \int_{B(x,R/2)} (u - \theta)_+^2 \, d\nu = 0.$$

In particular, it follows that $u(T,x) \le \theta$ and, hence, $u^2(T,x) \le \theta^2$. With an appropriate choice of θ, this will lead us to (8).

Applying Lemma 4 for two consecutive cylinders $\mathcal{C}_k \supset \mathcal{C}_{k+1}$ and using that

$$\theta_{k+1} - \theta_k = 2^{-(k+2)}\theta,$$

we obtain

$$J_{k+1} \le \frac{C J_k^{1+\beta}}{a\delta_k^{1+\beta} (\theta_{k+1} - \theta_k)^{2\beta}} = \frac{C' 4^{k\beta} J_k^{1+\beta}}{a\delta_k^{1+\beta}\theta^{2\beta}}, \tag{23}$$

where $C' = 16^{\beta} C$. Assume that δ_k is chosen so that for any k

$$\frac{C' 4^{-k\beta} J_0^{\beta}}{a\delta_k^{1+\beta}\theta^{2\beta}} = \frac{1}{16}. \tag{24}$$

We claim that then

$$J_k \le 16^{-k} J_0, \tag{25}$$

which in particular yields $J_k \to 0$. Indeed, for $k=0$ (25) is trivial. If (25) is true for some k then (23) and (24) imply

$$J_{k+1} \le \frac{C' 4^{k\beta} \left(16^{-k} J_0\right)^\beta}{a\delta_k^{1+\beta}\theta^{2\beta}} J_k = \frac{C' 4^{-k\beta} J_0^\beta}{a\delta_k^{1+\beta}\theta^{2\beta}} J_k \le \frac{1}{16}\left(16^{-k} J_0\right) = 16^{-(k+1)} J_0.$$

Resolving (24) with respect to δ_k we obtain

$$\delta_k = \left(\frac{16 C' 4^{-k\beta} J_0^\beta}{a\theta^{2\beta}}\right)^{\frac{1}{1+\beta}} = C'' \left(\frac{J_0^\beta}{a\theta^{2\beta}}\right)^{\frac{1}{1+\beta}} 4^{-\frac{k\beta}{1+\beta}}, \tag{26}$$

where $C'' = (16C')^{\frac{1}{1+\beta}}$. Note that any choice of δ_k determines uniquely the sequences $\{T_k\}$ and $\{R_k\}$, and these sequences should satisfy the requirements$T_k \le T/2$ and $R_k \ge R/2$. Since by (22)

$$T_k = \sum_{i=0}^{k-1} \delta_i \;\text{ and }\; R_k = R - \sum_{i=0}^{k-1} \sqrt{\delta_k},$$

the sequence $\{\delta_k\}$ must satisfy the inequalities

$$\sum_{k=0}^{\infty} \delta_k \le T/2 \text{ and } \sum_{k=0}^{\infty} \sqrt{\delta_k} \le R/2.$$

Substituting δ_k from (26) and observing that $\{\delta_k\}$ is a decreasing geometric sequence, we obtain that

$$\sum_{k=0}^{\infty} \delta_k = \left(\frac{J_0^\beta}{a\theta^{2\beta}}\right)^{\frac{1}{1+\beta}} \sum_{k=0}^{\infty} 4^{-\frac{k\beta}{1+\beta}} \le C''' \left(\frac{J_0^\beta}{a\theta^{2\beta}}\right)^{\frac{1}{1+\beta}}$$

and

$$\sum_{k=0}^{\infty} \sqrt{\delta_k} \le C''' \left(\frac{J_0^\beta}{a\theta^{2\beta}}\right)^{\frac{1}{2(1+\beta)}}$$

where C''' depends on β. Hence, the following inequalities must be satisfied:

$$\left(\frac{J_0^\beta}{a\theta^{2\beta}}\right)^{\frac{1}{1+\beta}} \le c^2 T \;\text{ and }\; \left(\frac{J_0^\beta}{a\theta^{2\beta}}\right)^{\frac{1}{2(1+\beta)}} \le cR,$$

for some $c = c(\beta) > 0$. There conditions can be satisfied by choosing θ as follows:

$$\theta^2 \ge \frac{a^{-1/\beta} J_0}{(c^2 T)^{1+1/\beta}} \text{ and } \theta^2 \ge \frac{a^{-1/\beta} J_0}{(cR)^{2+2/\beta}}.$$

Taking

$$\theta^2 = \frac{a^{-1/\beta} J_0}{c^{2(1+1/\beta)} \min\left(T, R^2\right)^{1+1/\beta}},$$

recalling that $u^2(T,x) \le \theta^2$ and using that

$$J_0 = \int_{\mathcal{C}_0} (u-\theta)_+^2 \, d\nu \le \int_{\mathcal{C}} u_+^2 d\nu,$$

we obtain

$$u^2(x,T) \le \frac{a^{-1/\beta}}{c^{2(1+1/\beta)} \min(T,R^2)^{1+1/\beta}} \int_{\mathcal{C}} u_+^2 d\nu,$$

whence (8) follows. ■

4 On-diagonal upper bounds

In what follows we frequently consider the Faber-Krahn inequality (4) with $\beta = 2/n$ (where $n > 0$ does not have to be the dimension of M). That is, we say that $\Omega \subset M$ satisfies the Faber-Krahn inequality with constant a if, for any $U \Subset \Omega$,

$$\lambda_{\min}(U) \ge a\mu(U)^{-2/n}. \tag{27}$$

Theorem 5 *Let a precompact ball $B(x,r)$ satisfy the Faber-Krahn inequality (27) with constant a. Then, for all $t > 0$,*

$$p_t(x,x) \le \frac{Ca^{-n/2}}{\min(t,r^2)^{n/2}}. \tag{28}$$

Proof. Since $p_t(x,x)$ is monotone decreasing in t, it suffices to prove (28) for $t \le r^2$.

The function

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

is a positive solution of the heat equation. Applying Theorem 2 in the cylinder $(t/2,t) \times B(x,r)$, we obtain

$$u^2(t,x) \le \frac{Ca^{-n/2}}{t^{1+n/2}} \int_{t/2}^{t} \int_{B(x,r)} u^2(s,y) \, d\mu(y) ds.$$

Observe that

$$\begin{aligned}\int_{t/2}^{t}\int_{B(x,r)} u^2(s,y)\,d\mu(y)ds &\le \int_{t/2}^{t}\int_{M} p_s^2(x,y)\,d\mu(y)ds \\ &= \int_{t/2}^{t} p_{2s}(x,x)\,ds \\ &\le \frac{t}{2} p_t(x,x),\end{aligned}$$

where we have used the semigroup identity and the fact that $p_s(x,x)$ is monotone decreasing in s. It follows that

$$p_t^2(x,x) \le \frac{Ca^{-n/2}t}{t^{1+n/2}} p_t(x,x)$$

which implies (28). ■

Example. Let M have bounded geometry, that is, there exists $r>0$ such that all balls $B(x,r)$ of radii r are uniformly quasi-isometric to the Euclidean ball of the same radius. Then the Faber-Krahn inequality (27) holds in any ball $B(x,r)$ with the same constant $a>0$ that does not depend on x. Hence, (28) holds on such manifolds for all $x\in M$ and $t>0$.

Theorem 6 *Let M be a geodesically complete manifold. The following conditions are equivalent:*

(a) *M satisfies the Faber-Krahn inequality (27) with some constant $a>0$.*

(b) *The heat kernel on M satisfies for all $x\in M$ and $t>0$ the inequality*

$$p_t(x,x)\leq Ct^{-n/2} \tag{29}$$

with some constant C.

Proof of Theorem 6 (a) $\Rightarrow$ (b)**.** By Theorem 5, (28) holds for an arbitrary r. Choosing $r\geq\sqrt{t}$, we obtain (29) for all $x\in M$ and $t>0$. ■

For the proof of the opposite implication (b) $\Rightarrow$ (a) we need the following lemma.

Lemma 7 *For any function $f\in C_0^\infty(M)$ such that $\|f\|_2=1$ and for any $t>0$, the following inequality holds*

$$\exp\left(-t\int_M|\nabla f|^2\,d\mu\right)\leq\|P_tf\|_2. \tag{30}$$

Consequently, for any open set $U\subset M$ and for any $t>0$,

$$\lambda_{\min}(U)\geq\frac{1}{t}\log\frac{1}{\sup\limits_{f\in\mathcal{T}(U)}\|P_tf\|_2}, \tag{31}$$

where

$$\mathcal{T}(U)=\left\{f\in C_0^\infty(U):\|f\|_2=1\right\}.$$

Proof. Let $\{E_\lambda\}_{\lambda\in\mathbb{R}}$ be the spectral resolution of the operator $\mathcal{L}=-\Delta$ in $L^2(M,\mu)$. Then, for any continuous function φ on $[0,\infty)$, we have

$$\varphi(\mathcal{L})=\int_0^\infty\varphi(\lambda)\,dE_\lambda$$

and, for any $f\in L^2(M,\mu)$,

$$\|\varphi(\mathcal{L})f\|_2^2=\int_0^\infty\varphi^2(\lambda)\,d\|E_\lambda f\|^2,$$

where the function $\lambda\mapsto\|E_\lambda f\|^2$ is monotone increasing.

For $\varphi\equiv1$ we have

$$\|f\|_2^2=\int_0^\infty d\|E_\lambda f\|^2,$$

and for $\varphi(\lambda) = e^{-t\lambda}$ we have

$$\|P_t f\|_2^2 = \|\exp(-t\mathcal{L}) f\|_2^2 = \int_0^\infty \exp(-2t\lambda)\, d\|E_\lambda f\|^2. \tag{32}$$

For $\varphi(\lambda) = \lambda^{1/2}$ and $f \in C_0^\infty(M)$ we have

$$\int_M |\nabla f|^2 \, d\mu = -\int_M (\Delta f) f \, d\mu = (\mathcal{L}f, f) = \left\|\mathcal{L}^{1/2} f\right\|_2^2 = \int_0^\infty \lambda d\|E_\lambda f\|^2. \tag{33}$$

If in addition $\|f\|_2 = 1$ then the measure $d\|E_\lambda f\|^2$ has the total mass 1. Applying Jensen's inequality, we obtain

$$\begin{aligned} \|P_t f\|_2^2 &= \int_0^\infty \exp(-2t\lambda)\, d\|E_\lambda f\|^2 \\ &\geq \exp\left(-\int_0^\infty 2t\lambda\, d\|E_\lambda f\|^2\right) \\ &= \exp\left(-2t \int_M |\nabla f|^2 \, d\mu\right), \end{aligned}$$

which is equivalent to (30).

Clearly, (30) implies

$$\int_M |\nabla f|^2 \, d\mu \geq \frac{1}{t} \log \frac{1}{\|P_t f\|_2}. \tag{34}$$

It follows from the variational property of $\lambda_{\min}(U)$ and (34) that

$$\begin{aligned} \lambda_{\min}(U) &= \inf_{f \in \mathcal{T}(U)} \int |\nabla f|^2 \, d\mu \\ &\geq \inf_{f \in \mathcal{T}(U)} \frac{1}{t} \log \frac{1}{\|P_t f\|_2} \\ &= \frac{1}{t} \log \frac{1}{\sup_{f \in \mathcal{T}(U)} \|P_t f\|_2}, \end{aligned}$$

which proves (31). ∎

Proof of Theorem 6 $(b) \Rightarrow (a)$**.** We have, for any $f \in L^2(M, \mu)$,

$$\begin{aligned} |P_t f(x)| &= \left| \int_M p_t(x,y) f(y) d\mu(y) \right| \\ &\leq \left(\int_M p_t^2(x,y)\, d\mu(y) \right)^{1/2} \|f\|_2 \\ &= p_{2t}(x,x)^{1/2} \|f\|_2 \end{aligned}$$

whence

$$\|P_t f(x)\|_\infty \leq C t^{-n/4} \|f\|_2.$$

It follows by the duality argument that for any $f \in L^2 \cap L^1$,

$$\begin{aligned} \|P_t f\|_2 &= \sup_{\|g\|_2 = 1} (P_t f, g) = \sup_{\|g\|_2 = 1} (f, P_t g) \\ &\leq \sup_{\|g\|_2 = 1} \|f\|_1 \|P_t g\|_\infty \\ &\leq C t^{-n/4} \|f\|_1, \end{aligned}$$

that is,

$$\|P_t f\|_2 \leq C t^{-n/4} \|f\|_1. \tag{35}$$

Let U be a precompact open subset of M and let $f \in \mathcal{T}(U)$, that is, $f \in C_0^\infty(U)$ and $\|f\|_2 = 1$. By the Cauchy-Schwarz inequality inequality, we have

$$\|f\|_1 \leq \sqrt{\mu(U)},$$

which together with (35) yields

$$\|P_t f\|_2 \leq C t^{-n/4} \sqrt{\mu(U)}.$$

By (31) we obtain, any $t > 0$,

$$\begin{aligned} \lambda_{\min}(U) &\geq \frac{1}{t} \log \frac{1}{\sup_{f \in \mathcal{T}(U)} \|P_t f\|_2} \\ &\geq \frac{1}{t} \log \frac{1}{C t^{-n/4} \sqrt{\mu(U)}}. \end{aligned}$$

Choose t here from the condition

$$C t^{-n/4} \sqrt{\mu(U)} = \frac{1}{e},$$

that is,

$$t = (Ce)^{4/n} \mu(U)^{2/n}.$$

It follows that

$$\lambda_{\min}(U) \geq \frac{1}{t} = a \mu(U)^{-2/n},$$

where $a = (Ce)^{-4/n}$, which finishes the proof. ■

5 A weighted L^2 norm of the heat kernel

The semigroup identity yields that

$$\int_M p_t(x,y)^2 \, d\mu(y) = \int_M p_t(x,y) \, p_t(y,x) \, d\mu(y) = p_{2t}(x,x),$$

which in particular implies that the function $p_t(x,\cdot)$ belongs to $L^2(M,\mu)$. In fact, a more interesting fact is true.

For any $D > 0$, consider the following weighted L^2 norm of the heat kernel:

$$E_D(t,x) = \int_M p_t^2(x,y) \exp\left(\frac{d^2(x,y)}{Dt}\right) d\mu(y), \tag{36}$$

where $d(x,y)$ is the geodesic distance on M. We can consider also the case $D = \infty$ by setting $\frac{1}{D} = 0$ so that

$$E_\infty(t,x) = p_{2t}(x,x).$$

Theorem 8 *(a) If $D \geq 2$ then $E_D(t,x)$ is non-increasing in t.*

(b) Let $B(x,r) \subset M$ be a relatively compact ball satisfying the Faber-Krahn inequality (27) with constant $a > 0$. Then, for any $t > 0$ and $D \in (2, +\infty]$,

$$E_D(t,x) \leq \frac{Ca^{-n/2}}{\min(t,r^2)^{n/2}}, \tag{37}$$

where $C = C(n,D)$.

(c) If $D > 2$ then $E_D(t,x) < \infty$.

Proof. (a) The following integrated maximum principle was proved in lectures in 2017: for any solution $u(t,y)$ of the heat equation on $I \times M$ (where I is a time interval) and for any locally Lipschitz function $\xi(t,y)$ in $I \times M$ satisfying

$$\partial_t \xi + \frac{1}{2}|\nabla \xi|^2 \leq 0,$$

the function

$$\int_M u^2(t,y)\, e^{\xi(t,y)} d\mu(y)$$

is non-increasing in $t \in I$. If $D \geq 2$ then the function

$$\xi(t,y) = \frac{d^2(x,y)}{Dt}$$

satisfies the inequality

$$\partial_t \xi + \frac{1}{2}|\nabla \xi|^2 \leq \partial_t \xi + \frac{D}{4}|\nabla \xi|^2 \leq 0,$$

and the latter is the case because

$$\xi_t = -\frac{d(x,y)^2}{Dt^2}, \quad |\nabla \xi|^2 \leq \frac{4d(x,y)^2}{D^2 t^2}.$$

Hence, $E_D(t,x)$ is non-increasing in t.

$(b)+(c)$ Note that $E_D(t,x)$ may be equal to ∞. For example, $E_2(t,x) = \infty$ in $\mathbb{R}^n$. The finiteness of $E_D(t,x)$ for $D > 2$ follows from the estimate (37) because for any $x \in M$ there is $r > 0$ such that $B(x,r)$ is relatively compact, and in any relatively compact domain the Faber-Krahn inequality always holds with some positive constant a.

Hence, it remains to prove (37). Since $E_D(t,x)$ is non-increasing in t and the right hand side of (37) is constant for $t > r^2$, it suffices to prove (37) for $t \leq r^2$, which will be assumed in the sequel.

Fix a non-negative function $f \in L^2(M)$ and set $u = P_t f$. Applying the mean value inequality of Theorem 2, we obtain

$$u^2(t,x) \leq K \int_0^t \int_{B(x,r)} u^2(s,y)\, d\mu(y)\, ds, \tag{38}$$

where

$$K=\frac{Ca^{-n/2}}{t^{1+n/2}}. \tag{39}$$

Set

$$\rho(y)=d(y,B(x,r))=(d(x,y)-r)_+$$

and consider the function

$$\xi(s,y)=-\frac{\rho^2(y)}{2(t-s)},$$

defined for $0\le s<t$ and $y\in M$. Since $\xi(y,s)\equiv 0$ for $y\in B(x,r)$ and, hence,

$$e^{\xi(y,s)}=1 \text{ for } y\in B(x,r),$$

we can rewrite (38) as follows:

$$u^2(t,x)\le K\int_0^t\int_M u^2(y,s)\,e^{\xi(y,s)}d\mu(y)\,ds. \tag{40}$$

Since

$$\partial_t\xi+\frac{1}{2}|\nabla\xi|^2\le 0,$$

by the integrated maximum principle, the function

$$J(s):=\int_M u^2(s,y)\,e^{\xi(s,y)}d\mu(y)$$

is non-increasing in $s\in[0,t)$. In particular, we have

$$J(s)\le J(0)\quad \text{for all } s\in[0,t).$$

It follows from (40) that

$$u^2(t,x)\le K\int_0^t J(s)\,ds\le KtJ(0).$$

Since

$$J(0)=\int_M f^2(y)\exp\left(-\frac{\rho^2(y)}{2t}\right)d\mu(y),$$

we obtain

$$u^2(t,x)\le Kt\int_M f^2(y)\exp\left(-\frac{\rho^2(y)}{2t}\right)d\mu(y). \tag{41}$$

Now choose function f as follows

$$f(y)=p_t(x,y)\exp\left(\frac{\rho^2(y)}{2t}\right)\varphi(y),$$

where φ is any function from $C_0^\infty(M)$ such that $0\le\varphi\le 1$. Then we have

$$u(t,x)=\int_M p_t(x,y)\,f(y)\,d\mu(y)=\int_M p_t^2(x,y)\exp\left(\frac{\rho^2(y)}{2t}\right)\varphi(y)\,d\mu(y).$$

Applying (41) with this function f and using that $\varphi^2 \leq \varphi$, we obtain

$$\begin{aligned} u^2(t,x) &\leq Kt \int_M p_t^2(x,y) \exp\left(\frac{\rho^2(y)}{t}\right) \varphi^2(y) \exp\left(-\frac{\rho^2(y)}{2t}\right) d\mu(y) \\ &\leq Kt \int_M p_t^2(x,y) \exp\left(\frac{\rho^2(y)}{2t}\right) \varphi(y)\, d\mu(y) \\ &= Kt\, u(t,x). \end{aligned}$$

It follows that

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

that is,

$$\int_M p_t^2(x,y) \exp\left(\frac{\rho^2(y)}{2t}\right) \varphi(y)\, d\mu(y) \leq Kt.$$

Since φ is arbitrary, we obtain that

$$\int_M p_t^2(x,y) \exp\left(\frac{\rho^2(y)}{2t}\right) d\mu(y) \leq Kt = C(at)^{-n/2}. \tag{42}$$

Using the elementary inequality[1]

$$\frac{a^2}{t} + \frac{b^2}{s} \geq \frac{(a+b)^2}{t+s}, \tag{43}$$

which is true for real a, b and positive t, s, we obtain, for any $D > 2$,

$$\frac{\rho^2(y)}{2t} + \frac{r^2}{(D-2)\,t} = \frac{(\rho(y)+r)^2}{Dt} \geq \frac{d^2(x,y)}{Dt}.$$

It follows that

$$\begin{aligned} E_D(t,x) &= \int_M p_t^2(x,y) \exp\left(\frac{d^2(x,y)}{Dt}\right) d\mu(y) \\ &\leq \exp\left(\frac{r^2}{(D-2)\,t}\right) \int_M p_t^2(x,y) \exp\left(\frac{\rho^2(y)}{2t}\right) d\mu(y). \end{aligned}$$

Note that we can always reduce r without changing the value of a. Since $r \geq \sqrt{t}$, we can set $r = \sqrt{t}$ and obtain

$$E_D(t,x) \leq \exp\left(\frac{1}{D-2}\right) C(at)^{-n/2},$$

which finishes the proof of (37). ■

[1] The inequality (43) follows from

$$\alpha X^2 + (1-\alpha)\,Y^2 \geq (\alpha X + (1-\alpha)\,Y)^2$$

for $\alpha = \frac{t}{t+s}$, $X = \frac{a}{\alpha}$ and $Y = \frac{b}{1-\alpha}$.

6 Gaussian upper estimates

Here we illustrate how one can obtain pointwise upper and lower bounds of the heat kernel by using the weighted norm $E_D(t,x)$.

Theorem 9 *Let two balls $B(x,r)$ and $B(y,r)$ be precompact and satisfy the Faber-Krahn inequality (27) with constants $a(x,r)$ and $a(y,r)$, respectively. Then, for all $t>0$ and $D>2$,*

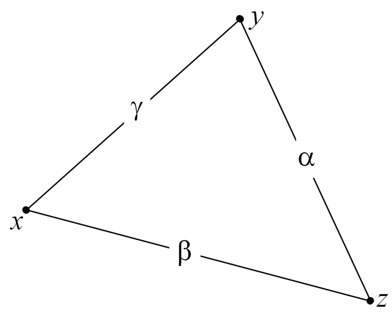
$$p_t(x,y) \le \frac{C}{(a(x,r)\,a(y,r))^{n/4}\min(t,r^2)^{n/2}}\exp\left(-\frac{d^2(x,y)}{2Dt}\right), \tag{44}$$

where $C = C(n,D)$.

Proof. Let us prove that always

$$p_{2t}(x,y) \le \sqrt{E_D(t,x)E_D(t,y)}\exp\left(-\frac{d^2(x,y)}{4Dt}\right). \tag{45}$$

Indeed, for any points $x,y,z \in M$, let us denote $\alpha = d(y,z)$, $\beta = d(x,z)$ and $\gamma = d(x,y)$.



Distances α,β,γ

By the triangle inequality, we have

$$\alpha^2+\beta^2 \ge \frac{1}{2}(\alpha+\beta)^2 \ge \frac{1}{2}\gamma^2.$$

Applying the semigroup identity (1), we obtain

$$\begin{aligned} p_{2t}(x,y) &= \int_M p_t(x,z)p_t(y,z)d\mu(z) \\ &\le \int_M p_t(x,z)e^{\frac{\beta^2}{2Dt}}p_t(y,z)e^{\frac{\alpha^2}{2Dt}}e^{-\frac{\gamma^2}{4Dt}}d\mu(z) \\ &\le \left(\int_M p_t^2(x,z)e^{\frac{\beta^2}{Dt}}d\mu(z)\right)^{\frac{1}{2}}\left(\int_M p_t^2(y,z)e^{\frac{\alpha^2}{Dt}}d\mu(z)\right)^{\frac{1}{2}}e^{-\frac{\gamma^2}{4Dt}} \\ &= \sqrt{E_D(t,x)E_D(t,y)}\exp\left(-\frac{d^2(x,y)}{4Dt}\right), \end{aligned}$$

which proves (45).

Combining (37) and (45), we obtain

$$p_{2t}(x,y) \le C\frac{\left(a(x,r)^{-n/2}a(y,r)^{-n/2}\right)^{1/2}}{\min(t,r^2)^{n/2}}\exp\left(-\frac{d^2(x,y)}{4Dt}\right)$$

which is equivalent to (44). ■

Example. Let M have bounded geometry, that is, there exists $r>0$ such that all balls $B(x,r)$ of radii r are uniformly quasi-isometric to the Euclidean ball of the same radius. Then the Faber-Krahn inequality (27) holds in any ball $B(x,r)$ with the constant a that does not depend on x. Hence, we obtain from (44), for all $t>0$ and $x,y\in M$,

$$p_t(x,y) \le \frac{C}{\min(t,r^2)^{n/2}}\exp\left(-\frac{d^2(x,y)}{2Dt}\right).$$

Corollary 10 *Let M satisfy the Faber-Krahn inequality (27) with some constant $a>0$. Then, for all $t>0$ and $x,y\in M$ and $D>2$,*

$$p_t(x,y) \le \frac{C}{t^{n/2}}\exp\left(-\frac{d^2(x,y)}{2Dt}\right), \tag{46}$$

where $C=C(a,n,D)$.

Proof. Indeed, by hypothesis (44) holds for any $r>0$. Setting $r=\sqrt{t}$, we obtain (46). ■

For example, (46) holds on Cartan-Hadamard manifolds.

It follows from Theorem 6 and Corollary 10 that the Gaussian estimate (46) holds if and only if the on-diagonal upper bound

$$p_t(x,y) \le \frac{C}{t^{n/2}}$$

is satisfied.

7 Li-Yau upper bounds

Set

$$V(x,r) = \mu(B(x,r)).$$

Definition. We say that M satisfies the volume doubling condition (or the measure μ is doubling) if, for all $x\in M$ and $r>0$,

$$V(x,2r) \le CV(x,r), \tag{47}$$

for some constant C.

Definition. We say that M satisfies the *relative Faber-Krahn inequality* (RFK) if any ball $B(x,r)$ on M satisfies the Faber-Krahn inequality (4) with some exponent $\beta > 0$ and with the constant

$$a = a(x,r) = b\frac{V(x,r)^\beta}{r^2} \tag{48}$$

where $b > 0$; that is, for any $U \Subset B(x,r)$,

$$\lambda_{\min}(U) \geq \frac{b}{r^2}\left(\frac{V(x,r)}{\mu(U)}\right)^\beta. \tag{49}$$

It is known that the relative Faber-Krahn inequality holds on complete manifolds of non-negative Ricci curvature. It holds also on any manifold $M = K \times \mathbb{R}^m$ where K is a compact manifold.

Theorem 11 *Let M be a complete, connected, non-compact manifold and fix $D > 2$. Then the following conditions are equivalent:*

(a) *M admits the relative Faber-Krahn inequality (49).*

(b) *The measure μ is doubling and the heat kernel satisfies the upper bound*

$$p_t(x,y) \leq \frac{C}{\left(V(x,\sqrt{t})\,V(y,\sqrt{t})\right)^{1/2}} \exp\left(-\frac{d(x,y)^2}{2Dt}\right), \tag{50}$$

for all for all $x,y \in M$, $t > 0$, and for some positive constant C.

(c) *The measure μ is doubling and the heat kernel satisfies the inequality*

$$p_t(x,x) \leq \frac{C}{V(x,\sqrt{t})}, \tag{51}$$

for all for all $x \in M$, $t > 0$, and for some constant C.

Remark. As we will see later, under any of the conditions (a)-(c) of Theorem 11 we have also the matching lower bound

$$p_t(x,x) \geq \frac{c}{V(x,\sqrt{t})},$$

for all $x \in M$, $t > 0$ and for some constant $c > 0$.

We precede the proof by two lemmas.

Lemma 12 *If a precompact ball $B(x,R)$ satisfies the Faber-Krahn inequality (4) with exponent β and constant a, then, for any $r < R$,*

$$V(x,r) \geq ca^{1/\beta}r^{2/\beta}, \tag{52}$$

where $c = c(\beta) > 0$.

Proof. Denote for simplicity $V(r) = V(x,r)$. Using the Lipschitz cutoff function φ of $B(x,r/2)$ in $B(x,r)$ as a test function in the variational property of the first eigenvalue, we obtain

$$\begin{aligned} V(r/2) &\leq \int_{B(x,r)} \varphi^2 d\mu \leq \lambda_{\min}(B(x,r))^{-1} \int_{B(x,r)} |\nabla\varphi|^2 d\mu \\ &\leq \left(aV(r)^{-\beta}\right)^{-1} \frac{4}{r^2} V(r) \\ &= \frac{4}{ar^2} V(r)^{1+\beta}, \end{aligned}$$

whence

$$V(r) \geq c\left(ar^2 V(r/2)\right)^{\theta},$$

where $\theta = \frac{1}{\beta+1}$ and $c = c(\beta) > 0$. Iterating this, we obtain

$$\begin{aligned} V(r) &\geq ca^{\theta} r^{2\theta} V\left(\frac{r}{2}\right)^{\theta} \\ &\geq c^{1+\theta} a^{\theta+\theta^2} r^{2\theta} \left(\frac{r}{2}\right)^{2\theta^2} V\left(\frac{r}{4}\right)^{\theta^2} \\ &\geq c^{1+\theta+\theta^2} a^{\theta+\theta^2+\theta^3} r^{2\theta} \left(\frac{r}{2}\right)^{2\theta^2} \left(\frac{r}{4}\right)^{2\theta^3} V\left(\frac{r}{8}\right)^{\theta^3} \\ &\quad ... \\ &\geq c^{1+\theta+\theta^2+...} a^{\theta\left(1+\theta+\theta^2+...\right)} r^{2\theta\left(1+\theta+\theta^2+...\right)} 2^{-2\theta^2\left(1+\theta+\theta^2+...\right)} V\left(\frac{r}{2^k}\right)^{\theta^k}, \end{aligned}$$

for any $k \in \mathbb{N}$. Observe that

$$V\left(\frac{r}{2^k}\right) \sim c_n \left(\frac{r}{2^k}\right)^n \quad \text{as } k \to \infty$$

and, hence, $V\left(\frac{r}{2^k}\right)^{\theta^k} \to 1$. Since

$$\theta\left(1+\theta+\theta^2+...\right) = \frac{\theta}{1-\theta} = \frac{1}{\beta},$$

we obtain as $k \to \infty$

$$V(r) \geq \text{const}\, a^{1/\beta} r^{2/\beta},$$

which was to be proved. ■

Lemma 13 *If M is connected, complete, non-compact and satisfies the doubling volume property then there are positive numbers ν, ν', c, C such that*

$$c\left(\frac{R}{r}\right)^{\nu'} \leq \frac{V(x,R)}{V(x,r)} \leq C\left(\frac{R}{r}\right)^{\nu} \tag{53}$$

for all $x \in M$ and $0 < r \leq R$. Besides, for all $x, y \in M$ and all $0 < r \leq R$,

$$\frac{V(x,R)}{V(y,r)} \leq C\left(\frac{R + d(x,y)}{r}\right)^{\nu}. \tag{54}$$

Proof. If $2^k r \leq R < 2^{k+1} r$ with a non-negative integer k then iterating the doubling property

$$V(x,2r) \leq CV(x,r),$$

we obtain

$$V(x,R) \leq V\left(x,2^{k+1}r\right) \leq C^{k+1}V(x,r) \leq C\left(\frac{R}{r}\right)^{\log_2 C} V(x,r),$$

so that the right inequality in (53) holds with $\nu = \log_2 C$.

The left inequality in (53) is called the *reverse volume doubling*. To prove it, assume first $R = 2r$. The connectedness of M implies that there is a point $y \in M$ such that $d(x,y) = \frac{3}{2}r$. Then $B\left(y, \frac{1}{2}r\right) \leq B(x,2r) \setminus B(x,r)$, which implies

$$V(x,2r) \geq V(x,r) + V(y,\frac{1}{2}r).$$

By (47), we have

$$\frac{V(x,r)}{V(y,\frac{1}{2}r)} \leq \frac{V(y,4r)}{V\left(y,\frac{1}{2}r\right)} \leq C^3,$$

whence

$$V(x,2r) \geq \left(1+C^{-3}\right)V(x,r).$$

Iterating this inequality, we obtain (53) with $\nu' = \log_2(1+C^{-3})$.

Finally, (54) follows from (53) as follows:

$$\frac{V(x,R)}{V(y,r)} \leq \frac{V(y,R+d(x,y))}{V(y,r)} \leq C\left(\frac{R+d(x,y)}{r}\right)^{\nu}.$$

■

Proof of Theorem 11. $(a) \implies (b)$ Choose n so that $\beta = 2/n$. By Theorem 9 we have, for all $x,y \in M$ and $r,t>0$,

$$p_t(x,y) \leq \frac{C}{\left(a(x,r)\,a(y,r)\min(t,r^2)\min(t,r^2)\right)^{n/4}}\exp\left(-\frac{\rho^2}{2Dt}\right).$$

Choosing $r = \sqrt{t}$ and substituting a from (48) we obtain

$$\begin{aligned} p_t(x,y) &\leq \frac{C}{\left(V\left(x,\sqrt{t}\right)^{2/n}V\left(y,\sqrt{t}\right)t^{-2}\right)^{n/4}t^{n/2}}\exp\left(-\frac{d^2(x,y)}{2Dt}\right) \\ &= \frac{C}{\left(V\left(x,\sqrt{t}\right)V\left(y,\sqrt{t}\right)\right)^{1/2}}\exp\left(-\frac{d^2(x,y)}{2Dt}\right). \end{aligned}$$

that is (50).

It remains to prove that μ is doubling. Applying Lemma 12 with

$$a = b\frac{V(x,R)^{\beta}}{R^2},$$

we obtain

$$V(x,r) \geq c\left(\frac{r}{R}\right)^{2/\beta} V(x,R), \tag{55}$$

whence the doubling property follows.

$(b) \implies (c)$ Trivial: just set $x=y$ in (50).

$(c) \implies (a)$ Fix a ball $B(x,r)$ and consider an open set $U \subset B(x,r)$. We have, for all $y \in U$,

$$p_t^U(y,y) \leq p_t(y,y) \leq \frac{C}{V\left(y,\sqrt{t}\right)}.$$

For any $y \in U$ and $t \leq r^2$, we have by the volume doubling

$$\frac{V(x,r)}{V\left(y,\sqrt{t}\right)} \leq \frac{V(y,2r)}{V\left(y,\sqrt{t}\right)} \leq C\left(\frac{r}{\sqrt{t}}\right)^{\nu},$$

so that, for $t \leq r^2$,

$$p_t^U(y,y) \leq \frac{C}{V(x,r)}\left(\frac{r}{\sqrt{t}}\right)^{\nu}.$$

As in the proof of Theorem 6, it follows that, for all $f \in L^2(U)$,

$$\left\|P_t^U f\right\|_2^2 \leq \frac{C}{V(x,r)}\left(\frac{r}{\sqrt{t}}\right)^{\nu}\|f\|_1^2.$$

Let $f \in C_0^\infty(U)$ be a function such that $\|f\|_2 = 1$. Since by the Cauchy-Schwarz inequality

$$\|f\|_1^2 \leq \mu(U),$$

we obtain by Lemma 7 that

$$\begin{aligned}
\lambda_{\min}(U) &\geq \frac{1}{2t}\log\frac{1}{\sup\limits_{f\in\mathcal{T}(U)}\left\|P_t^U f\right\|_2^2} \\
&\geq \frac{1}{2t}\log C^{-1}\frac{V(x,r)}{\mu(U)}\left(\frac{\sqrt{t}}{r}\right)^{\nu}.
\end{aligned}$$

Now choose t from the condition

$$C^{-1}\left(\frac{\sqrt{t}}{r}\right)^{\nu}\frac{V(x,r)}{\mu(U)} = e, \tag{56}$$

that is,

$$t = \left(\frac{Ce\mu(U)}{V(x,r)}\right)^{2/\nu} r^2.$$

Since we need to have $t \leq r^2$, we have to assume for a while that

$$\mu(U) \leq (Ce)^{-1} V(x,r). \tag{57}$$

If so then we obtain from above that

$$\lambda_{\min}(U) \geq \frac{1}{2t} = \frac{b}{r^2}\left(\frac{V(x,r)}{\mu(U)}\right)^{2/\nu}. \tag{58}$$

where $b>0$ is a positive constant, which was to be proved.

We are left to extend (58) to any $U \Subset B(x,r)$ without the restriction (57). For that, we will use Lemma 13. Find $R>r$ so big that

$$\frac{V(x,R)}{V(x,r)} \geq Ce,$$

Due to (53), we can take R in the form $R=Ar$, where A is a constant, depending on the other constants in question. Then $U \subset B(x,R)$ and

$$\mu(U) \leq (Ce)^{-1} V(x,R),$$

which implies by the first part of the proof that

$$\lambda_1(U) \geq \frac{b}{R^2}\left(\frac{V(x,R)}{\mu(U)}\right)^{2/\nu} \geq \frac{b}{(Ar)^2}\left(\frac{V(x,r)}{\mu(U)}\right)^{2/\nu},$$

which was to be proved. ■

Using (54), we obtain

$$\frac{V\left(x,\sqrt{t}\right)}{V\left(y,\sqrt{t}\right)} \leq C\left(\frac{\sqrt{t}+d(x,y)}{\sqrt{t}}\right)^{\nu} = C\left(1+\frac{d(x,y)}{\sqrt{t}}\right)^{\nu}.$$

Replacing $V\left(y,\sqrt{t}\right)$ in (50) according to this inequality, we obtain

$$p_t(x,y) \leq \frac{C}{V\left(x,\sqrt{t}\right)} \exp\left(-\frac{d^2(x,y)}{2D't}\right), \tag{59}$$

where $D'>D$. Since $D>2$ was arbitrary, we see that $D'>2$ is also arbitrary.

The estimate (59) for manifolds of non-negative Ricci curvature was proved by P.Li and S.-T. Yau in 1986. In fact, they also proved a matching lower bound in this case.

8 On-diagonal lower estimates of the heat kernel

Now let us discuss some on-diagonal *lower* bound of the heat kernel.

Theorem 14 *Let M be a geodesically complete Riemannian manifold. Assume that, for some $x \in M$ and all $r \geq r_0$,*

$$V(x,r) \leq Cr^{\nu}, \tag{60}$$

where C,ν,r_0 are positive constants. Then, for all $t \geq t_0$,

$$p_t(x,x) \geq \frac{1/4}{V(x,\sqrt{\eta t \log t})}, \tag{61}$$

where $\eta = \eta(x,r_0,C,\nu) > 0$ and $t_0 = \max(r_0^2, 3)$.

Of course, (61) implies that, for large t,

$$p_t(x,x) \geq c\,(t\log t)^{-\nu/2}.$$

There are examples to show that in general one cannot get rid of $\log t$ here.

Proof. For any $r>0$, we obtain by the semigroup identity and the Cauchy-Schwarz inequality

$$\begin{aligned} p_{2t}(x,x) &= \int_M p_t^2(x,\cdot)d\mu \geq \int_{B(x,r)} p_t^2(x,\cdot)d\mu \\ &\geq \frac{1}{V(x,r)}\left(\int_{B(x,r)} p_t(x,\cdot)d\mu\right)^2. \end{aligned} \tag{62}$$

By (60) the manifold M is stochastically complete, that is

$$\int_M p_t(x,\cdot)d\mu = 1.$$

Since $p_t(x,x) \geq p_{2t}(x,x)$, it follows from (62) that

$$p_t(x,x) \geq \frac{1}{V(x,r)}\left(1 - \int_{M\setminus B(x,r)} p_t(x,\cdot)d\mu\right)^2. \tag{63}$$

Choose $r=r(t)$ so that

$$\int_{M\setminus B(x,r(t))} p_t(x,\cdot)d\mu \leq \frac{1}{2}. \tag{64}$$

Then (63) yields

$$p_t(x,x) \geq \frac{1/4}{V(x,r(t))}.$$

Hence, we obtain (61) provided

$$r(t) = \sqrt{\eta t \log t}. \tag{65}$$

It remains to prove the following: there exists a large enough η such that, for any $t \geq t_0$, the inequality (64) holds with the function $r(t)$ from (65).

Setting $\rho = d(x,\cdot)$ and fixing some $D>2$ (for example, $D=3$), we obtain by the Cauchy-Schwarz inequality

$$\begin{aligned} \left(\int_{M\setminus B(x,r)} p_t(x,\cdot)d\mu\right)^2 &\leq \int_M p_t^2(x,\cdot)\exp\left(\frac{\rho^2}{Dt}\right)d\mu \int_{M\setminus B(x,r)} \exp\left(-\frac{\rho^2}{Dt}\right)d\mu \\ &= E_D(t,x)\int_{M\setminus B(x,r)} \exp\left(-\frac{\rho^2}{Dt}\right)d\mu, \end{aligned} \tag{66}$$

where $E_D(t,x)$ is defined by (36). By Theorem 8, we have, for all $t \geq t_0$,

$$E_D(t,x) \leq E_D(t_0,x) < \infty. \tag{67}$$

Since x is fixed, we can consider $E_D(t_0, x)$ as a constant.

Let us now estimate the integral in (66) assuming that

$$r = r(t) \geq r_0. \tag{68}$$

By splitting the complement of $B(x,r)$ into the union of the annuli

$$B(x, 2^{k+1}r) \setminus B(x, 2^k r), \quad k = 0, 1, 2, ...,$$

and using the hypothesis (60), we obtain

$$\int_{M\setminus B(x,r)} \exp\left(-\frac{\rho^2}{Dt}\right) d\mu \leq \sum_{k=0}^{\infty} \exp\left(-\frac{4^k r^2}{Dt}\right) V(x, 2^{k+1}r) \tag{69}$$

$$\leq Cr^\nu \sum_{k=0}^{\infty} 2^{\nu(k+1)} \exp\left(-\frac{4^k r^2}{Dt}\right). \tag{70}$$

Assuming further that

$$\frac{r^2(t)}{Dt} \geq 1, \tag{71}$$

we see that the sum in (70) is majorized by a geometric series, whence

$$\int_{M\setminus B(x,r)} \exp\left(-\frac{\rho^2}{Dt}\right) d\mu \leq C' r^\nu \exp\left(-\frac{r^2}{Dt}\right), \tag{72}$$

where C' depends on C and ν.

Both conditions (68) and (71) are satisfies for $r(t) = \sqrt{\eta t \log t}$, if

$$t \geq t_0 = \max\left(r_0^2, 3\right)$$

and η is large enough, say $\eta > 1$ and $\eta > D$. Substituting (65) into (72), we obtain

$$\int_{M\setminus B(x,r)} \exp\left(-\frac{\rho^2}{Dt}\right) d\mu \leq C' (\eta t \log t)^{\nu/2} \exp\left(-\frac{\eta \log t}{D}\right)$$

$$= C' \eta^{\nu/2} \left(\frac{\log t}{t^{\frac{2\eta}{\nu D}-1}}\right)^{\nu/2}. \tag{73}$$

Note that the function $\frac{\log t}{t}$ is decreasing for $t \geq e$. Hence, assuming further that $\eta \geq \nu D$ we obtain from (73) and (66) that, for $t \geq t_0$,

$$\left(\int_{M\setminus B(x,r)} p_t(x,\cdot) d\mu\right)^2 \leq C' \eta^{\nu/2} \left(\frac{\log t_0}{t_0^{\frac{2\eta}{\nu D}-1}}\right)^{\nu/2} E_D(t_0, x). \tag{74}$$

Finally, choosing η large enough, we can make the right hand side arbitrarily small, which finishes the proof of (64). ■

Theorem 15 *Let M be a complete, connected, non-compact manifold that satisfies the relative Faber-Krahn inequality (49). Then, for all $t > 0$ and $x \in M$,*

$$p_t(x,x) \geq \frac{c}{V\left(x,\sqrt{t}\right)} \tag{75}$$

for some $c = c(b,\beta)$.

Proof. As it was proved in Theorem 11, the measure μ is doubling, which, in particular, implies that M is stochastically complete. Following the argument in the proof of Theorem 14, we need to find $r = r(t)$ so that

$$\int_{M\setminus B(x,r)} p_t(x,\cdot)d\mu \leq \frac{1}{2},$$

which implies

$$p_t(x,x) \geq \frac{1/4}{V(x,r(t))}. \tag{76}$$

If in addition $r(t) \leq K\sqrt{t}$ for some constant K then (75) follows from (76) and the doubling property of μ.

Let us use the estimate (66) from the proof of Theorem 14, that is,

$$\left(\int_{M\setminus B(x,r)} p_t(x,\cdot)d\mu\right)^2 \leq E_D(t,x)\int_{M\setminus B(x,r)} \exp\left(-\frac{d^2(x,\cdot)}{Dt}\right)d\mu \tag{77}$$

where $D > 2$ (for example, set $D = 3$). Next, instead of using the monotonicity of $E_D(t,x)$ as in the proof of Theorem 14, we apply Theorem 8 which yields, for all $x \in M$ and $t, R > 0$, that

$$E_D(t,x) \leq \frac{Ca(x,R)^{-1/\beta}}{\min(t,R^2)^{1/\beta}} = \frac{C\left(b\frac{V(x,R)^\beta}{R^2}\right)^{-1/\beta}}{\min(t,R^2)^{1/\beta}} = \frac{C'}{V(x,R)\min\left(t/R^2,1\right)^{1/\beta}}.$$

Choosing here $R = \sqrt{t}$, we obtain

$$E_D(t,x) \leq \frac{C}{V(x,\sqrt{t})}. \tag{78}$$

Applying the doubling property, we obtain

$$\begin{aligned}
\int\limits_{M\setminus B(x,r)} \exp\left(-\frac{d^2(x,\cdot)}{Dt}\right)d\mu &\leq \sum_{k=0}^{\infty}\exp\left(-\frac{4^k r^2}{Dt}\right)V(x,2^{k+1}r) \\
&\leq \sum_{k=0}^{\infty} C^{k+1}\exp\left(-\frac{4^k r^2}{Dt}\right)V(x,r) \\
&\leq C'V(x,r)\exp\left(-\frac{r^2}{Dt}\right), \qquad (79)
\end{aligned}$$

provided $r^2 \geq Dt$. It follows from (77), (78), ,(79) and (53) that

$$\left(\int_{M \setminus B(x,r)} p_t(x,\cdot)d\mu\right)^2 \leq C'' \frac{V(x,r)}{V\left(x,\sqrt{t}\right)} \exp\left(-\frac{r^2}{Dt}\right)$$
$$\leq C\left(\frac{r}{\sqrt{t}}\right)^{\nu} \exp\left(-\frac{r^2}{Dt}\right).$$

Obviously, the right hand side here can be made arbitrarily small by choosing $r = \sqrt{\eta t}$ with η large enough, which finishes the proof. ■

9 Upper Gaussian bounds via on-diagonal estimates

We say that a function $\gamma : (0, +\infty) \to (0, +\infty)$ is regular if it is monotone increasing and satisfies the doubling conditions: there is $A \geq 1$ such that for all $t > 0$,

$$\gamma(2t) \leq A\gamma(t). \tag{80}$$

Theorem 16 *Let M be a Riemannian manifold and $S \subset M$ be a a non-empty measurable subset of M. For any function $f \in L^2(M)$ and $t > 0$ and $D > 0$ set*

$$E_D(t,f) = \int_M (P_t f)^2 \exp\left(\frac{d^2(\cdot,S)}{Dt}\right) d\mu. \tag{81}$$

Assume that, for some $f \in L^2(S)$ and for all $t > 0$,

$$E_\infty(t,f) = \|P_t f\|_2^2 \leq \frac{1}{\gamma(t)}, \tag{82}$$

where $\gamma(t)$ is a regular function on $(0, +\infty)$. Then, for all $D > 2$ and $t > 0$,

$$E_D(t,f) \leq \frac{6A}{\gamma(ct)}, \tag{83}$$

where $c = c(D) > 0$.

In the proof we use the Davies-Gaffney inequality in the following form: for any measurable set $A \subset M$, any function $h \in L^2(M)$ and for all positive ρ, τ,

$$\int_{A_\rho^c} (P_\tau h)^2 d\mu \leq \int_{A^c} h^2 d\mu + \exp\left(-\frac{\rho^2}{2\tau}\right) \int_A h^2 d\mu, \tag{84}$$

where S_ρ denotes the open ρ-neighborhood of S.

Proof. The proof will be split into four steps.

Step 1. Set for any $r, t > 0$

$$J_r(t) := \int_{S_r^c} (P_t f)^2 d\mu.$$

Let $R > r > 0$ and $T > t > 0$. Applying (84) with $h = P_t f$, $A = S_r$, $\tau = T - t$ and $\rho = R - r$, we obtain

$$\int_{S_R^c} (P_T f)^2 \, d\mu \leq \int_{S_r^c} (P_t f)^2 \, d\mu + \exp\left(-\frac{(R-r)^2}{2(T-t)}\right) \int_{S_r} (P_t f)^2 \, d\mu.$$

By (82), we have

$$\int_{S_r} (P_t f)^2 \, d\mu \leq \frac{1}{\gamma(t)},$$

whence it follows that

$$J_R(T) \leq J_r(t) + \frac{1}{\gamma(t)} \exp\left(-\frac{(R-r)^2}{2(T-t)}\right). \tag{85}$$

Step 2. Let us prove that

$$J_r(t) \leq \frac{3A}{\gamma(t/2)} \exp\left(-\varepsilon \frac{r^2}{t}\right), \tag{86}$$

for some $\varepsilon > 0$. Let $\{r_k\}_{k=0}^{\infty}$ and $\{t_k\}_{k=0}^{\infty}$ be two strictly decreasing sequences of positive reals such that

$$r_0 = r, \quad r_k \downarrow 0, \quad t_0 = t, \; t_k \downarrow 0$$

as $k \to \infty$. By (85), we have, for any $k \geq 1$,

$$J_{r_{k-1}}(t_{k-1}) \leq J_{r_k}(t_k) + \frac{1}{\gamma(t_k)} \exp\left(-\frac{(r_{k-1} - r_k)^2}{2(t_{k-1} - t_k)}\right). \tag{87}$$

When $k \to \infty$ we obtain

$$J_{r_k}(t_k) = \int_{S_{r_k}^c} (P_{t_k} f)^2 \, d\mu \leq \int_{S^c} (P_{t_k} f)^2 \, d\mu \to \int_{S^c} f^2 d\mu = 0, \tag{88}$$

where we have used the fact that $P_t f \to f$ in $L^2(M)$ as $t \to 0+$ and the hypothesis that $f \equiv 0$ in S^c.

Adding up the inequalities (87) for all k from 1 to ∞ and using (88), we obtain

$$J_r(t) \leq \sum_{k=1}^{\infty} \frac{1}{\gamma(t_k)} \exp\left(-\frac{(r_{k-1} - r_k)^2}{2(t_{k-1} - t_k)}\right). \tag{89}$$

Let us specify the sequences $\{r_k\}$ and $\{t_k\}$ as follows:

$$r_k = \frac{r}{k+1} \quad \text{and} \quad t_k = 2^{-k} t.$$

For all $k \geq 1$ we have

$$r_{k-1} - r_k = \frac{r}{k(k+1)} \quad \text{and} \quad t_{k-1} - t_k = 2^{-k} t,$$

whence

$$\frac{(r_{k-1}-r_k)^2}{2(t_{k-1}-t_k)} = \frac{2^k}{2k^2(k+1)^2}\frac{r^2}{t} \geq \varepsilon(k+1)\frac{r^2}{t}$$

where

$$\varepsilon = \inf_{k\geq 1}\frac{2^k}{2k^2(k+1)^3} > 0. \tag{90}$$

By the condition (80) we have

$$\frac{\gamma(t_{k-1})}{\gamma(t_k)} \leq A,$$

which implies

$$\frac{\gamma(t)}{\gamma(t_k)} = \frac{\gamma(t_0)}{\gamma(t_1)}\frac{\gamma(t_1)}{\gamma(t_2)}\dots\frac{\gamma(t_{k-1})}{\gamma(t_k)} \leq A^k.$$

Substituting into (89), we obtain

$$\begin{aligned} J_r(t) &\leq \frac{1}{\gamma(t)}\sum_{k=1}^{\infty} A^k \exp\left(-\varepsilon(k+1)\frac{r^2}{t}\right) \\ &= \frac{\exp\left(-\varepsilon\frac{r^2}{t}\right)}{\gamma(t)}\sum_{k=1}^{\infty}\exp\left(kL-\varepsilon k\frac{r^2}{t}\right), \end{aligned}$$

where

$$L := \log A.$$

Consider the following two cases:

1. If $\varepsilon\frac{r^2}{t} - L \geq 1$ then

$$J_r(t) \leq \frac{\exp\left(-\varepsilon\frac{r^2}{t}\right)}{\gamma(t)}\sum_{k=1}^{\infty}\exp(-k) \leq \frac{2}{\gamma(t)}\exp\left(-\varepsilon\frac{r^2}{t}\right).$$

2. If $\varepsilon\frac{r^2}{t} - L < 1$ then we estimate $J_r(t)$ in a trivial way:

$$J_r(t) \leq \int_M (P_t f)^2\, d\mu \leq \frac{1}{\gamma(t)},$$

   whence

$$\begin{aligned} J_r(t) &\leq \frac{1}{\gamma(t)}\exp\left(1+L-\varepsilon\frac{r^2}{t}\right) = \frac{e}{\gamma(t)}A\frac{\gamma(t_0)}{\gamma(t_1)}\exp\left(-\varepsilon\frac{r^2}{t}\right) \\ &\leq \frac{3A}{\gamma(t/2)}\exp\left(-\varepsilon\frac{r^2}{t}\right). \end{aligned}$$

Hence, in the both cases we obtain (86).

Step 3. Let us prove the inequality

$$E_D(t,f) \leq \frac{6A}{\gamma(t/2)} \tag{91}$$

under the additional restriction that

$$D \geq 5\varepsilon^{-1}, \tag{92}$$

where ε was defined by (90) in the previous step.

Set $\rho(x) = d(x, S)$ and split the integral in the definition (81) of $E_D(t, f)$ into the series

$$E_D(t, f) = \left(\int_{\{\rho \leq r\}} + \sum_{k=1}^{\infty} \int_{\{2^{k-1}r < \rho \leq 2^k r\}} \right) (P_t f)^2 \exp\left(\frac{\rho^2}{Dt}\right) d\mu, \tag{93}$$

where r is a positive number to be chosen below. The integral over the set $\{\rho \leq r\}$ is estimated using (82):

$$\begin{aligned} \int_{\{\rho \leq r\}} (P_t f)^2 \exp\left(\frac{\rho^2}{Dt}\right) d\mu &\leq \exp\left(\frac{r^2}{Dt}\right) \int_M (P_t f)^2 \, d\mu \\ &\leq \frac{1}{\gamma(t)} \exp\left(\frac{r^2}{Dt}\right). \end{aligned} \tag{94}$$

The k-th term in the sum in (93) is estimated by (86) as follows

$$\begin{aligned} &\int_{\{2^{k-1}r < \rho \leq 2^k r\}} (P_t f)^2 \exp\left(\frac{\rho^2}{Dt}\right) d\mu \\ \leq \; & \exp\left(\frac{4^k r^2}{Dt}\right) \int_{S^c_{2^{k-1}r}} (P_t f)^2 \, d\mu \\ = \; & \exp\left(\frac{4^k r^2}{Dt}\right) J_{2^{k-1}r}(t) \\ \leq \; & \frac{3A}{\gamma(t/2)} \exp\left(\frac{4^k r^2}{Dt} - \varepsilon \frac{4^{k-1} r^2}{t}\right) \\ \leq \; & \frac{3A}{\gamma(t/2)} \exp\left(-\frac{4^{k-1} r^2}{Dt}\right), \end{aligned} \tag{95}$$

where in the last line we have used (92).

Let us choose $r = \sqrt{Dt}$. Then we obtain from (93), (94), and (95)

$$E_D(t, f) \leq \frac{3}{\gamma(t)} + \sum_{k=1}^{\infty} \frac{3A}{\gamma(t/2)} \exp\left(-4^{k-1}\right) \leq \frac{3 + 3A}{\gamma(t/2)},$$

whence (91) follows.

Step 4. We are left to prove (83) in the case

$$2 < D < D_0 := 5\varepsilon^{-1}. \tag{96}$$

By Theorem 8, we have for any $s > 0$ and all $0 < \tau < t$

$$\int_M (P_t f)^2 \exp\left(\frac{\rho^2}{2(t+s)}\right) d\mu \leq \int_M (P_\tau f)^2 \exp\left(\frac{\rho^2}{2(\tau+s)}\right) d\mu. \tag{97}$$

Given $t>0$ and D as in (96), let us choose the values of s and τ so that the left hand side of (96) be equal to $E_D(t,f)$ whereas the right hand side be equal to $E_{D_0}(\tau,f)$. In other words, s and τ must satisfy the simultaneous equations

$$\begin{cases} 2(t+s)=Dt, \\ 2(\tau+s)=D_0\tau, \end{cases}$$

whence we obtain

$$s=\frac{D-2}{2}t \quad \text{and} \quad \tau=\frac{D-2}{D_0-2}t<t.$$

Hence, we can rewrite (97) in the form

$$E_D(t,f)\leq E_{D_0}(\tau,f).$$

By (91), we have

$$E_{D_0}(\tau,f)\leq\frac{6A}{\gamma(2^{-1}\tau)},$$

whence we conclude

$$E_D(t,f)\leq\frac{6A}{\gamma(\frac{D-2}{D_0-2}2^{-1}t)},$$

thus finishing the proof of (83). ■

Theorem 17 *If, for some $x\in M$ and all $t>0$,*

$$p_t(x,x)\leq\frac{1}{\gamma(t)},$$

where γ is a regular function on $(0,+\infty)$ then, for all $D>2$ and $t>0$,

$$E_D(t,x)\leq\frac{6A}{\gamma(ct)}, \tag{98}$$

where $c=c(D)>0$ and A is the constant from (80).

Proof. Let U be an open relatively compact neighborhood of the point x, and let φ be a cutoff function of $\{x\}$ in U. For any $s>0$ define the function φ_s on M by

$$\varphi_s(z)=p_s(x,z)\varphi(z).$$

Clearly, we have $\varphi_s\leq p_s(x,\cdot)$ whence

$$P_t\varphi_s\leq P_tp_s(x,\cdot)=p_{t+s}(x,\cdot)$$

and

$$\|P_t\varphi_s\|_2^2\leq\|p_{t+s}(x,\cdot)\|_2^2\leq\|p_t(x,\cdot)\|_2^2=p_{2t}(x,x)\leq\frac{1}{\gamma(2t)}.$$

By Theorem 16, we conclude that, for any $D>2$,

$$\int_M(P_t\varphi_s)^2\exp\left(\frac{d^2(\cdot,U)}{Dt}\right)d\mu\leq\frac{6A}{\gamma(ct)}. \tag{99}$$

Fix $y \in M$ and observe that, by the definition of φ_s,

$$P_t\varphi_s(y) = \int_M p_t(y,z)\, p_s(x,z)\, \varphi(z)\, d\mu(z) = P_s\psi_t(x),$$

where

$$\psi_t(z) := p_t(y,z)\varphi(z)$$

Since function $\psi_t(\cdot)$ is continuous and bounded, we conclude that

$$P_s\psi_t(x) \to \psi_t(x) \text{ as } s \to 0,$$

that is,

$$P_t\varphi_s(y) \to p_t(x,y) \quad \text{as } s \to 0.$$

Passing to the limit in (99) as $s \to 0$, we obtain by Fatou's lemma

$$\int_M p_t^2(x,\cdot) \exp\left(\frac{d^2(\cdot,U)}{Dt}\right) d\mu \leq \frac{6A}{\gamma(ct)}.$$

Finally, shrinking U to the point x, we obtain (98). ■

Corollary 18 *Let γ_1 and γ_2 be two regular functions on $(0,+\infty)$, and assume that, for two points $x,y \in M$ and all $t>0$*

$$p_t(x,x) \leq \frac{1}{\gamma_1(t)} \quad \text{and} \quad p_t(y,y) \leq \frac{1}{\gamma_2(t)}.$$

Then, for all $D>2$ and $t>0$,

$$p_t(x,y) \leq \frac{6A}{\sqrt{\gamma_1(ct)\gamma_2(ct)}} \exp\left(-\frac{d^2(x,y)}{2Dt}\right),$$

where A is the constant from (80) and $c = c(D) > 0$.

Proof. By Theorem 17, we obtain

$$E_D(t,x) \leq \frac{6A}{\gamma_1(ct)} \quad \text{and} \quad E_D(t,y) \leq \frac{6A}{\gamma_2(ct)}.$$

Substituting these inequalities into the estimate (45), we finish the proof. ■

In particular, if

$$p_t(x,x) \leq \frac{1}{\gamma(t)}$$

for all $x \in M$ and $t>0$ then

$$p_t(x,y) \leq \frac{C}{\gamma(ct)} \exp\left(-\frac{d^2(x,y)}{2Dt}\right),$$

for all $x,y \in M$ and $t>0$. If the manifold M is complete and $\gamma(t) = ct^{n/2}$ then this follows also from Theorem 6 and Corollary 10.

At the end, let us show how Theorem 17 allows to obtain a lower estimate of the heat kernel.

Theorem 19 *Let M be a complete manifold. Assume that, for some point $x \in M$ and all $r > 0$*

$$V(x, 2r) \le CV(x, r),$$

and, for all $t > 0$,

$$p_t(x, x) \le \frac{C}{V(x, \sqrt{t})}. \tag{100}$$

Then, for all $t > 0$,

$$p_t(x, x) \ge \frac{c}{V(x, \sqrt{t})},$$

where $c > 0$ depends on C.

Proof. The proof goes in the same way as that of Theorem 15. In the proof of Theorem 15 we have used the relative Faber-Krahn inequality in order to obtain (78), that is,

$$E_D\left(t, x\right) \le \frac{C}{V\left(x, \sqrt{t}\right)}.$$

However, in the present setting, this inequality follows directly from (100) by Theorem 17. The rest of the proof of Theorem 15 goes unchanged. ■