Estimates of heat kernels on Riemannian manifolds

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1 Introduction

The purpose of these notes is to give introduction to the subject of heat kernels on non-compact Riemannian manifolds. By definition, the heat kernel for the Euclidean space $\mathbb{R}^n$ is the (unique) positive solution of the following Cauchy problem in $(0, +\infty) \times \mathbb{R}^n$

$$\begin{cases} \frac{\partial u}{\partial t} = \Delta u \,, \\ u(0, x) = \delta(x - y), \end{cases}$$

where $u = u(t, x)$ and $y \in \mathbb{R}^n$. It is denoted by $p(t, x, y)$ and is given by the classical formula

$$p(t, x, y) = \frac{1}{(4\pi t)^{n/2}} \exp\left(-\frac{|x - y|^2}{4t}\right). \tag{1.1}$$

In other words, $p(t, x, y)$ is a positive fundamental solution to the heat equation $\frac{\partial u}{\partial t} = \Delta u$. This means, in particular, that the Cauchy problem

$$\begin{cases} \frac{\partial u}{\partial t} = \Delta u, \\ u(0, t) = f(x) \end{cases}$$

is solved by

$$u(t, x) = \int_{\mathbb{R}^n} p(t, x, y) f(y) dy,$$

provided f is a bounded continuous function.

Another definition of the heat kernel (which justifies the letter p) is as follows: it is the transition density of the Brownian motion in $\mathbb{R}^n$ (up to the change of time $t \to t/2$). Given that much, it is not surprising that the heat kernel plays a central role in potential theory in $\mathbb{R}^n$.

Consider now an arbitrary smooth connected Riemannian manifold M. There is a natural generalization of the Laplace operator linked to the Riemannian structure of M. It is called the Riemannian Laplace operator or the Laplace-Beltrami operator and is also denoted by Δ. It turns out that the notion of the heat kernel can be defined on any manifold. Let us denote it also by $p(t, x, y)$, where $t > 0$ and $x, y \in M$. However, explicit formulas for $p(t, x, y)$ exist only for a few classes of manifolds possessing enough symmetries. The simplest explicit heat kernel formula after (1.1) is one for the three-dimensional hyperbolic space $\mathbb{H}^3$ which reads as follows

$$p(t, x, y) = \frac{1}{(4\pi t)^{3/2}} \exp\left(-\frac{d^2}{4t} - t\right) \frac{d}{\sinh d}, \tag{1.2}$$

where $d = d(x, y)$ is the geodesic distance between $x, y \in \mathbb{H}^3$. Clearly, there is certain similarity between (1.1) and (1.2) (note that $|x - y|$ is the geodesic distance in $\mathbb{R}^n$) but there are also two distinctions: the terms $\exp(-t)$ and $\frac{d}{\sinh d}$ in (1.2). They reflect the difference between the geometries of the Euclidean and hyperbolic spaces.

It turns out that the heat kernel is rather sensitive to the geometry of manifolds, which makes the study of the heat kernel interesting and rich from the geometric point of view. On the other hand, there are the properties of the heat kernel which little depend on the geometry and reflect rather structure of the heat equation. For example, the presence of the Gaussian exponential term $\exp\left(-\frac{d^2}{4t}\right)$ in the heat kernel estimates is one of such features.

Most part of these notes is devoted to the heat kernel upper estimates on arbitrary manifolds. We discuss both general techniques of obtaining the heat kernel bounds, presented in Sections 3, 5, 6, and their applications for particular classes of manifolds, in Section 7. In Section 4, we apply the heat kernel bounds to estimate eigenvalues of the Laplace operator. Many results are supplied with proofs whose purpose is to demonstrate the underlying ideas rather than to achieve the full generality.

We do not aim at a detailed account of lower estimates of the heat kernel and touch only one aspect of those in Section 5.3, not the least because this subject is so far not well understood. Other results on the lower bounds of heat kernel on manifolds can be found in [15], [28], [67], [78], [98], [110], [120], [123].

We have to skip some other interesting questions related to the heat kernels such as the Harnack inequality [67], [68], [98], [120], [121], comparison theorems [28], [52], short time asymptotics [62], [85], [105], [112], [119], [131], estimates of time derivatives of the heat kernel [44], [49], [71], gradient estimates [82], [86], [98], [100], [125], [117], [138], [141], discretization techniques [24], [25], [34], [88], homogenization techniques [2], [11], [90], [110], etc. Finally, we do not treat heat kernels on underlying spaces other than Riemannian manifolds and for operators other than the Laplace operator. See the following references for heat kernels

- on symmetric spaces [3];
- on groups and Lie groups [1], [13], [14], [108], [118], [135];
- for random walks on graphs [30], [53], [79], [83], [89], [114], [136];
- for second order elliptic operators with lower order terms [40], [59], [99], [107], [111], [123], [137];
- for higher order elliptic operators [6], [47], [48];
- for subelliptic operators [11], [12], [91], [92];
- for non-linear p-harmonic Laplacian [54];
- for Laplacian on exterior differential forms [56], [57], [58];
- for abstract local Dirichlet forms [127], [128];
- for Brownian motion on fractals [7], [8], [9], [10].

Needless to say that this list of references is very far from being complete.

Notation. The letters C, c and their modifications C', c', C_1, c_1 etc. are used for positive constants which may be different in different context.

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2 Construction of the heat kernel on manifolds

2.1 Laplace operator

The Laplace operator in $\mathbb{R}^n$ is defined by

$$\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial^2 X^i}$$

where X^1, X^2,..., X^n are the Cartesian coordinates. In order to write down the Laplace operator in an arbitrary curvilinear coordinate system x^1, x^2,..., x^n let us first note that the length element

$$ds^2 = \left(dX^1\right)^2 + \left(dX^2\right)^2 + ... + \left(dX^n\right)^2$$

takes in the coordinates x^1, x^2,..., x^n the following form

$$ds^2 = \sum_{i,j=1}^{n} g_{ij}(x) dx^i dx^j \tag{2.1}$$

where (g_{ij}) is a symmetric positive definite matrix. The change of variables in Δ gives then

$$\Delta = \frac{1}{\sqrt{g}} \sum_{i,j=1}^{n} \frac{\partial}{\partial x^i} \left(\sqrt{g} g^{ij} \frac{\partial}{\partial x^j} \right) \tag{2.2}$$

where $g := \det(g_{ij})$ and $\left(g^{ij}\right) = (g_{ij})^{-1}$.

Let M be an arbitrary smooth connected n-dimensional Riemannian manifold M. In general, there is no selected coordinate system on M but one can still define the Laplace operator in any chart $x^1, x^2, ..., x^n$ by using (2.2), where g_{ij} is now the Riemannian metric tensor on M (which determines the length by (2.1)). The definition (2.2) is covariant, that is, in any other chart this operator will have the same form. Hence, Δ is defined on all of M. The Laplace operator can also be represented as $\Delta = \mathrm{div}\nabla$, where the gradient ∇ and the divergence div are defined by

$$(\nabla u)^i = \sum_{j=1}^{n} g^{ij} \frac{\partial u}{\partial x^j}$$

and

$$\mathrm{div} F = \frac{1}{\sqrt{g}} \sum_{i,j=1}^{n} \frac{\partial}{\partial x^i} \left(\sqrt{g} F^i \right).$$

The Riemannian structure allows to introduce on M volumes of all dimensions. Particularly important for us will be the Riemannian n-volume μ defined by

$$d\mu = \sqrt{g} dx^1 dx^2 ... dx^3.$$

The Stokes's theorem implies the following integration-by-parts formula

$$\int_\Omega v \Delta u \, d\mu = -\int_\Omega (\nabla u, \nabla v) \, d\mu, \tag{2.3}$$

where Ω is a pre-compact open subset of M, u and v are C^2 functions in Ω such that one of them vanishes in a neighborhood of the boundary $\partial\Omega$, and $(\cdot, \cdot)$ means the inner product of the vector fields induced by the Riemannian tensor. More generally, if $u, v \in C^1\left(\overline{\Omega}\right) \cap C^2(\Omega)$ and $\partial\Omega \in C^1$ then

$$\int_\Omega v \Delta u \, d\mu = \int_{\partial\Omega} v \frac{\partial u}{\partial \nu} d\sigma - \int_\Omega (\nabla u, \nabla v) \, d\mu, \tag{2.4}$$

where σ is the surface area, that is, the $(n-1)$-dimensional Riemannian measure on M, and ν is the outward normal vector field on $\partial\Omega$.

See [22] and [119] for a detailed account of the notions of Riemannian geometry related to the Laplace operator.

2.2 Eigenvalues and eigenfunctions of the Laplace operator

Given a precompact open set $\Omega \subset M$, consider the Dirichlet eigenvalue problem in Ω

$$\begin{cases} \Delta u + \lambda u = 0, \\ u|_{\partial\Omega} = 0. \end{cases} \tag{2.5}$$

To be exact, we should define a weak solution to (2.5). Consider the spaces

$$L^2(\Omega) := \left\{ f : \int_\Omega f^2 d\mu < \infty \right\},$$

$$W_1^2(\Omega) := \left\{ f \in L^2(\Omega) : |\nabla f| \in L^2(\Omega) \right\},$$

where ∇f is understood in the sense of distributions, and define $\overset{o}{H}_1(\Omega)$ to be the closure of $C_0^\infty(\Omega)$ in $W_1^2(\Omega)$.

We define a weak solution to (2.5) as a function $u \in \overset{o}{H}_1(\Omega)$ that satisfies the equation $\Delta u + \lambda u = 0$ in the sense of distributions. The latter can be shown to be equivalent to the integral identity

$$\int_\Omega (\nabla u, \nabla v)\, d\mu = \lambda \int uv d\mu, \quad \forall v \in \overset{o}{H}_1(\Omega).$$

The standard technique of the spectral theory of elliptic operators implies that there exists an orthonormal basis $\{\phi_k\}_{k=1}^\infty$ in $L^2(\Omega)$ such that each ϕ_k is a weak eigenvalue of Δ in Ω with an eigenvalue $\lambda_k = \lambda_k(\Omega)$, and

$$0 \le \lambda_1 \le \lambda_2 \le ... \le \lambda_k \underset{k\to\infty}{\longrightarrow} \infty.$$

If Ω is connected then $\lambda_1(\Omega)$ is a single eigenvalue, that is, $\lambda_2(\Omega) > \lambda_1(\Omega)$, and $\phi_1(x) \neq 0$ in Ω. It is also possible to prove that if $M \setminus \overline{\Omega}$ is non-empty then $\lambda_1(\Omega) > 0$. On the other hand, if M is compact then we may take $\Omega = M$ in which case $\lambda_1(M) = 0$, with the eigenfunction $\phi_1(x) \equiv \mu(M)^{-1/2} = \text{const}$, but $\lambda_2(M) > 0$.

The operator Δ can be considered as a unbounded operator in $L^2(\Omega)$, with the domain $C_0^\infty(\Omega)$. As such, it turns out to be essentially self-adjoint. Its closure is called the Dirichlet Laplace operator and will be denoted by Δ_Ω. It has the domain

$$Dom(\Delta_\Omega) = \left(f \in \overset{o}{H}_1(\Omega) : \Delta f \in L^2(\Omega) \right)$$

and the spectrum $spec(-\Delta_\Omega) = \{\lambda_k\}_{k=1}^\infty$ (it is sometimes convenient to refer to $-\Delta_\Omega$ rather than to Δ_Ω because the former is positive definite). Clearly, in the basis $\{\phi_k\}$ the operator $-\Delta_\Omega$ is represented by the (infinite) diagonal matrix

$$-\Delta_\Omega = diag\,(\lambda_1, \lambda_2, ..., \lambda_k, ...)\,.$$

By the spectral theory, one can define $f(-\Delta_\Omega)$ where f is a function on $spec\,(-\Delta_\Omega)$. Particularly important is the operator $\exp(t\Delta_\Omega)$ where t is a real parameter. In the basis $\{\phi_k\}$, it has the matrix

$$\exp(t\Delta_\Omega) = diag\left(e^{-t\lambda_1}, e^{-t\lambda_2}, ..., e^{-t\lambda_k}, ...\right). \tag{2.6}$$

Hence, if $t \ge 0$ then $\exp(t\Delta_\Omega)$ is a bounded self-adjoint operator in $L^2(\Omega)$.

2.3 Heat kernel in precompact regions

Consider the following initial-boundary problem in $(0,\infty) \times \Omega$

$$\begin{cases} \frac{\partial u}{\partial t} = \Delta u, \\ u(0,x) = f(x), \\ u(t,x)|_{x\in\partial\Omega} = 0. \end{cases} \tag{2.7}$$

We understand it in a weak sense, as an evolution equation in $L^2(\Omega)$. Namely, we interpret $u(t,x)$ as a function from $[0,\infty)$ to $L^2(\Omega)$ such that

1. u is Fréchet differentiable in $t > 0$ and its Fréchet derivative $\dot{u}$ is equal to Δu (which, in particular, means that $\Delta u \in L^2(\Omega)$);

2. u is L^2-continuous at $t = 0$ and $u(0,\cdot) = f$;

3. for each $t > 0$, $u(t,\cdot) \in \overset{o}{H}_1(\Omega)$.

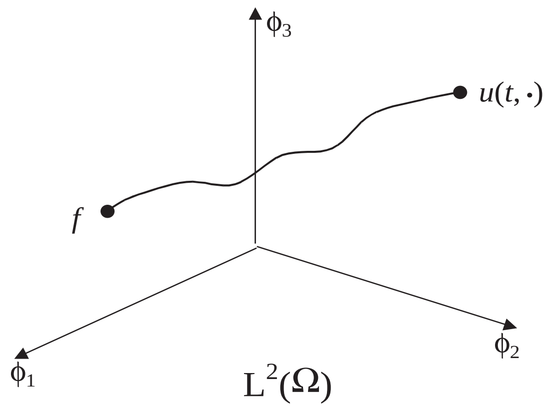

Figure 1 Function $u(t,x)$ as a path in $L^2(\Omega)$

It is easy to verify that the evolution equation $\dot{u} = \Delta u$ has solution

$$u = e^{t\Delta_\Omega} f. \tag{2.8}$$

Let us write this down in the basis $\{\phi_k\}$. The function $f \in L^2(\Omega)$ has the following expansion in this basis

$$f = \sum_{k=1}^{\infty} a_k \phi_k$$

where

$$a_k = \int_\Omega f(y)\phi_k(y)d\mu(y)\,.$$

Then, by (2.6),

$$\begin{aligned} e^{t\Delta_\Omega} f(x) &= \sum_{k=1}^{\infty} a_k e^{-t\lambda_k(\Omega)}\phi_k(x) \\ &= \sum_{k=1}^{\infty} e^{-t\lambda_k(\Omega)}\phi_k(x)\int_\Omega f(y)\phi_k(y)d\mu(y) \\ &= \int_\Omega \left\{\sum_{k=1}^{\infty} e^{-t\lambda_k(\Omega)}\phi_k(x)\phi_k(y)\right\} f(y)d\mu(y). \end{aligned}$$

The kernel in the curly brackets is called the heat kernel of Ω and will be denoted by $p_\Omega(t,x,y)$. Hence, we have

$$p_\Omega(t,x,y) := \sum_{k=1}^{\infty} e^{-t\lambda_k(\Omega)}\phi_k(x)\phi_k(y) \tag{2.9}$$

and the weak solution $u(t,x)$ to (2.7) is given by

$$u(t,x) = e^{t\Delta_\Omega} f = \int_\Omega p_\Omega(t,x,y)f(y)d\mu(y). \tag{2.10}$$

Note that (2.10) is just another way to write down (2.8). Hence, the operator $e^{t\Delta_\Omega}$ has the integral kernel $p_\Omega(t,x,y)$.

The eigenfunction $\phi_k(x)$ are C^∞-smooth, by the local elliptic regularity. The sequence $\{\lambda_k\}$ obeys Weyl's asymptotic formula

$$\lambda_k(\Omega) \sim c_n \left(\frac{k}{\mu(\Omega)}\right)^{2/n}, \quad k \to \infty,$$

and, hence, is growing fast enough to ensure convergence of (2.9) locally in any $C^m(\Omega)$. Hence, $p_\Omega \in C^\infty((0,\infty)\times\Omega\times\Omega)$. The solution $u(t,x)$ defined by (2.10) is then C^∞-smooth and satisfies the heat equation in the classical sense. If f is continuous then it is possible to show that $u(t,x)$ is continuous in the classical sense in $[0,\infty)\times\Omega$ and $u(t,x)=f(x)$.

Since $\phi_k \in \overset{o}{H}_1(\Omega)$, we obtain that p_Ω is also in $\overset{o}{H}_1(\Omega)$ as a function of x (or y). If the boundary $\partial\Omega$ is smooth, then this implies that $p_\Omega(t,x,y)$ extends continuously to $\overline{\Omega}$ and that p_Ω vanishes on $\partial\Omega$. In particular, the function u defined by (2.10) is also continuous on $(0,\infty)\times\partial\Omega$ and $u(t,x)=0$ for all $t>0$ and $x\in\partial\Omega$.

Other simple properties of p_Ω are as follows:

(a) As a function of t and x, the function $p_\Omega(t,x,y)$ satisfies the heat equation

$$\frac{\partial p_\Omega}{\partial t} = \Delta p_\Omega$$

and the initial value

$$p_\Omega(t,\cdot,y) \to \delta_y \quad \text{as} \quad t\to 0+ \ .$$

(b) The semigroup property: for all $t,s>0$ and $x,y\in\Omega$,

$$p_\Omega(t+s,x,y) = \int_\Omega p_\Omega(t,x,z)p_\Omega(s,x,y)d\mu(z), \tag{2.11}$$

which is another way to write down the identity $e^{(t+s)\Delta_\Omega} = e^{t\Delta_\Omega}e^{s\Delta_\Omega}$.

(c) The symmetry

$$p_\Omega(t,x,y) = p_\Omega(t,y,x). \tag{2.12}$$

The latter is obvious from (2.9) but would not be so transparent if we were to define p_Ω as a kernel which solves the initial-boundary problem (2.7) by (2.10).

If Ω is connected and $M\setminus\overline{\Omega}$ is non-empty then $\lambda_1(\Omega)>0$ is a single eigenvalue, $\phi_1(x)\neq 0$ in Ω, and (2.9) implies

$$p_\Omega(t,x,y) \sim e^{-t\lambda_1(\Omega)}\phi_1(x)\phi_1(y), \quad t\to\infty. \tag{2.13}$$

If M is compact then we may take $\Omega = M$ in which case (2.9) yields

$$p_M(t,x,y) = \frac{1}{\mu(M)} + \sum_{k=2}^{\infty} e^{-t\lambda_k(M)}\phi_k(x)\phi_k(y). \tag{2.14}$$

In particular, we have

$$p_M(t,x,y) \to \mu(M)^{-1}, \quad t\to\infty. \tag{2.15}$$

2.4 Maximum principle and positivity of the heat kernel

The properties of the heat kernel p_Ω discussed above follows from the self-adjointness of the Laplace operator in $L^2(\Omega)$. However, there is another aspect of the Laplace operator which cannot be derived only from the spectral properties. For example, it is known that $p_\Omega(t,x,y)>0$ for all $t>0$ and $x,y\in\Omega$. However, the positivity of the heat kernel is not at all obvious from the eigenfunction expansion (2.9), because the eigenfunctions ϕ_k are signed (except for ϕ_1).

Here we consider another property of the heat equation which is called the maximum (minimum) principle and which is responsible for the positivity of the heat kernel. Denote $\Omega_T = (0,T)\times\Omega$, which is a cylinder in $[0,\infty)\times M$, and define its *parabolic boundary* $\partial_p\Omega_T$ by

$$\partial_p\Omega_T := \partial\Omega_T \setminus \{(t,x) : t = T\}.$$

In other words, $\partial_p\Omega_T$ is the part of the boundary $\partial\Omega$ without the top of the cylinder.

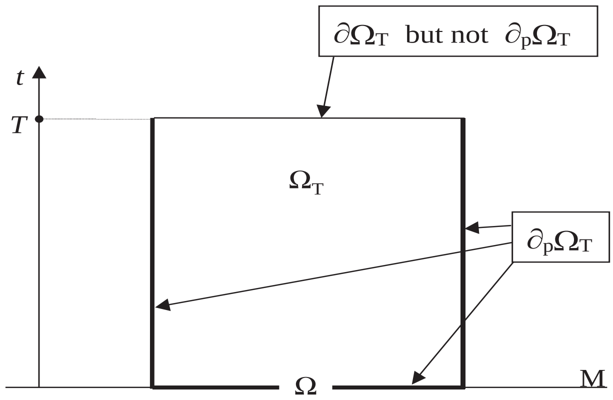

Figure 2 The parabolic boundary $\partial_p \Omega_T$

Proposition 2.1 *(The maximum/minimum principle) Let $u(t,x) \in C^2(\Omega_T) \cap C(\overline{\Omega})$ solve the heat equation in Ω_T. Then*

$$\sup_{\Omega_t} u = \sup_{\partial_p \Omega_T} u \tag{2.16}$$

and

$$\inf_{\Omega_T} u = \inf_{\partial_p \Omega_T} u\,. \tag{2.17}$$

If the initial function f in the initial-boundary problem (2.7) is non-negative then the minimum principle (2.17) implies that a (classical) solution $u(t,x)$ of (2.7) should be non-negative, too. If $\partial\Omega$ is smooth then the function $u = e^{t\Delta_\Omega} f$ is a classical solution to (2.7) whence

$$e^{t\Delta_\Omega} f \geq 0, \quad \forall f \in C_0^\infty(\Omega),\ f \geq 0.$$

Therefore, the kernel p_Ω of the operator $e^{t\Delta_\Omega}$ must be non-negative. By applying the strong version of the minimum principle, one can show that, in fact, p_Ω must be strictly positive in $(0,\infty) \times \Omega$.

A non-smooth boundary $\partial\Omega$ can be handled, too. However, we will always assume that $\partial\Omega$ is smooth if this simplifies the argument.

Another consequence of the maximum principle is the inequality

$$e^{t\Delta_\Omega} 1 \leq 1. \tag{2.18}$$

Indeed, $u = e^{t\Delta_\Omega} 1$ solves the problem (2.7) with $f \equiv 1$ and, obviously, $\sup_{\partial_p \Omega_T} u \leq 1$. Hence, by (2.16), we have $\sup_{\Omega_T} u \leq 1$ which means $u \leq 1$ everywhere. Clearly, (2.18) and (2.10) imply

$$\int_\Omega p_\Omega(t,x,y) d\mu(y) \leq 1. \tag{2.19}$$

The third consequence of the maximum principle is the monotonicity of p_Ω with respect to Ω: if $\Omega \subset \Omega'$, where Ω' is also a precompact open subset of M then

$$p_\Omega(t,x,y) \leq p_{\Omega'}(t,x,y). \tag{2.20}$$

Of course, one should specify the range of t,x,y in (2.20). If we extend $p_\Omega(t,x,y)$ by 0 for $x,y \notin \Omega$ then (2.20) holds for all $t > 0$ and $x,y \in M$.

Let us sketch the proof of (2.20). For any function $f \in C_0^\infty(\Omega)$, $f \geq 0$, we compare the functions $u = e^{t\Delta_\Omega} f$ and $u' = e^{t\Delta_{\Omega'}} f$ in Ω_T. Both have the same initial datum, but on the boundary $\partial\Omega$, we have $u(t,x) = 0 \leq u'(t,x)$. Hence,

$$\inf_{\partial_p \Omega_T} (u' - u) \geq 0,$$

and the minimum principle (2.17) implies $u' - u \geq 0$ in Ω_T and $u' \geq u$. Clearly, $e^{t\Delta_{\Omega'}} f \geq e^{t\Delta_\Omega} f$ implies $p_{\Omega'} \geq p_\Omega$, which was to be proved.

2.5 Heat semigroup on a manifold

The monotonicity of the heat kernel p_Ω with respect in Ω allows to construct the heat kernel p on the entire manifold M by taking the limit as "$\Omega \to M$". The latter means that we consider an exhaustion sequence $\{\Omega_k\}$ that is a sequence of precompact open sets $\Omega_k \subset M$ such that $\partial\Omega_k$ is smooth, $\overline{\Omega_k} \subset \Omega_{k+1}$ and

$$\bigcup_{k=1}^{\infty} \Omega_k = M.$$

Such sequence can be constructed on any manifold. Then we define

$$p(t,x,y) := \lim_{k\to\infty} p_{\Omega_k}(t,x,y). \tag{2.21}$$

Since $p_{\Omega_{k+1}} \geq p_{\Omega_k}$, the limit exists (finite or infinite) and does not depend on the choice of $\{\Omega_k\}$. As follows from (2.19),

$$\int_M p(t,x,y)d\mu(y) \leq 1,$$

so that p is finite almost everywhere. By the convergence properties of solutions to the parabolic equations, $p(t,x,y)$ is finite everywhere and C^∞-smooth.

Clearly, $p(t,x,y)$ inherits all previously discussed properties of $p_\Omega(t,x,y)$ except for the eigenfunction expansion (2.9). Moreover, it is possible to define the Dirichlet extension of the Laplace operator Δ on M (denote it Δ_M) and to show that $p(t,x,y)$ is the kernel of the semigroup $e^{t\Delta_M}$ acting in $L^2(M)$ (see [55]). However, the spectrum of Δ_M is not necessarily discrete as for a precompact region Ω. This is why it is not possible in general to define the heat kernel by the eigenfunction expansion (2.9).

After the heat kernel has been constructed by (2.21), we can give a shorter definition.

Definition 2.2 *The heat kernel $p(t,x,y)$ on M is the smallest positive fundamental solution to the heat equation on $(0,\infty)\times M$.*

A "fundamental solution" means that

$$\begin{cases} \frac{\partial p}{\partial t} = \Delta_x p, \\ p(t,\cdot,y) \underset{t\to 0}{\longrightarrow} \delta_y. \end{cases} \tag{2.22}$$

If $q(t,x,y)$ is another positive fundamental solution then the minimum principle implies $q \geq p_\Omega$ for any precompact region Ω. By (2.21), we obtain $q \geq p$ and p is the smallest one.

The purpose of all constructions in this section was to provide the (sketch of) proof of the existence of the smallest positive fundamental solution and to obtain its most important properties. The full justification of the above constructions can be found in [55], [22].

As an example of application, let us consider a direct Riemannian product $M = M' \times M''$ where M' and M'' are Riemannian manifolds. It is easy to see that $\Delta = \Delta' + \Delta''$ and $\mu = \mu' \times \mu''$, where the dashes refer to the manifolds M' and M'', respectively. The heat kernel on M is also a direct product of the heat kernels in M' and M'', that is,

$$p(t,x,y) = p'(t,x',y')p''(t,x'',y''), \tag{2.23}$$

where $x = (x',x'') \in M$ and $y = (y',y'') \in M$. Indeed, one first proves the obvious modification of (2.23) for a precompact region $\Omega = \Omega' \times \Omega'' \subset M$ directly by (2.9), and then passes to the limit as in (2.21).

In particular, the heat kernel (1.1) in $\mathbb{R}^n$ can be obtained from the heat kernel in $\mathbb{R}^1$ by iterating (2.23). If $M' = \mathbb{R}^m$ and $M'' = K$ where K is a compact manifold then, by (2.23), (1.1) and (2.15), the heat kernel on $M = \mathbb{R}^m \times K$ has the following asymptotic

$$p(t,x,x) \sim \mu''(K)^{-1}(4\pi t)^{-m/2}, \quad t \to \infty. \tag{2.24}$$

3 Integral estimates of the heat kernel

In this section, we introduce an integral version of the maximum principle and apply it to estimate some integrals of the heat kernel.

3.1 Integral maximum principle

Lemma 3.1 *(Aronson [4]) Let $\Omega \subset M$ be a precompact region. Suppose that $u(t,x) \in C^2\left(\overline{\Omega_T}\right)$ solves the heat equation in Ω_T and satisfies the boundary condition $u|_{\partial\Omega} = 0$. Let $\xi(t,x)$ be a locally Lipschitz function on $(0,\infty) \times M$ such that*

$$\xi_t + \frac{1}{2}|\nabla \xi|^2 \leq 0. \tag{3.1}$$

Then the function

$$J(t) := \int_\Omega u^2(t,x) e^{\xi(t,x)} d\mu(x) \tag{3.2}$$

is non-increasing in t.

Why is this called a maximum principle? Indeed, assume $u \geq 0$ and consider another function

$$S(t) = \sup_{x\in\Omega} u(t,x).$$

By applying (2.16) in $\Omega_{s,t} := (s,t) \times \Omega$ where $t > s > 0$, we obtain

$$S(s) = \sup_{\partial_p \Omega_{s,t}} u = \sup_{\Omega_{s,t}} u \geq S(t),$$

that is, $S(t)$ is non-increasing.

It is possible to prove that the following function

$$S_\alpha(t) = \|u(\cdot,t)\|_{L^\alpha(\Omega)}$$

is non-increasing for all $\alpha \in [1,\infty]$. If $\alpha = 2$ then this amounts to Lemma 3.1 with $\xi \equiv 0$. Hence, Lemma (3.1) is a weighted version of the fact that $S_2(t)$ is non-increasing, whereas the classical maximum principle implies that $S_\infty(t)$ is non-increasing.

Non-trivial examples of function ξ satisfying (3.1) are as follows:

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

and

$$\xi(t,x) = ad(x) - \frac{a^2}{2}t, \quad a \in \mathbb{R},$$

provided $d(x)$ is a Lipschitz function such that

$$|\nabla d| \leq 1.$$

Proof of Lemma 3.1. Let us differentiate $J(t)$ and show that $J' \leq 0$. Indeed, we have, by using $\xi_t \leq -\frac{1}{2}|\nabla\xi|^2$, $u_t = \Delta u$ and by (2.3),

$$\begin{aligned}
J'(t) &= \int_\Omega u^2 \xi_t e^\xi + 2\int_\Omega u u_t e^\xi \\
&\leq -\frac{1}{2}\int_\Omega u^2 |\nabla\xi|^2 e^\xi + 2\int_\Omega u\Delta u\, e^\xi \\
&= -\frac{1}{2}\int_\Omega u^2 |\nabla\xi|^2 e^\xi - 2\int_\Omega u\left(\nabla u, \nabla\xi\right) e^\xi - 2\int_\Omega |\nabla u|^2\, e^\xi \\
&= -\frac{1}{2}\int_\Omega \left(u\nabla\xi + 2\nabla u\right)^2 e^\xi,
\end{aligned} \tag{3.3}$$

which is non-positive. ■

One can get from (3.3) a sharper estimate for the decay of $J(t)$. Indeed, let us observe that

$$\frac{1}{2}\left(u\nabla\xi + 2\nabla u\right)^2 e^{\xi} = 2|\nabla(ue^{\xi/2})|^2.$$

By the variational property of $\lambda_1(\Omega)$,

$$\int_\Omega |\nabla(ue^{\xi/2})|^2 d\mu \geq \lambda_1(\Omega)\int_\Omega |ue^{\xi/2}|^2 = \lambda_1(\Omega)\, J(t).$$

Hence, (3.3) yields $J' \leq -2\lambda_1(\Omega)\, J$ whence

$$J(t) \leq J(t_0)\exp\left(-2\lambda_1(\Omega)(t-t_0)\right), \quad \forall t \geq t_0 > 0. \tag{3.4}$$

If $\xi(t,x) \equiv 0$ and $u(t,x) = p_\Omega(t,x,x_0)$ then, by (2.12) and (2.11),

$$J(t) = \int_\Omega p_\Omega^2(t,x,x_0)d\mu(x) = p_\Omega(2t,x_0,x_0).$$

Therefore, as a consequence of Lemma 3.1, $p_\Omega(t,x_0,x_0)$ is non-increasing in t. By letting $\Omega \nearrow M$ we see that $p(t,x_0,x_0)$ is non-increasing in t either.

3.2 The Davies inequality

The following theorem shows why the Gaussian exponential term is relevant to the heat kernel upper bounds on arbitrary manifolds.

Theorem 3.2 *(Davies [45]) Let M be an arbitrary Riemannian manifold and let A and B be two μ-measurable sets on M. Then*

$$\int_A\int_B p(t,x,y)d\mu(x)d\mu(y) \leq \sqrt{\mu(A)\mu(B)}\exp\left(-\frac{d^2(A,B)}{4t}\right), \tag{3.5}$$

where $d(A,B)$ is the geodesic distance between A and B (if A and B intersect then $d(A,B)=0$).

The first proof. By the approximation argument, it suffices to prove (3.5) for compact A and B. Furthermore, if A and B are compact then it suffices to prove (3.5) for the heat kernel p_Ω of any precompact open set Ω containing A and B.

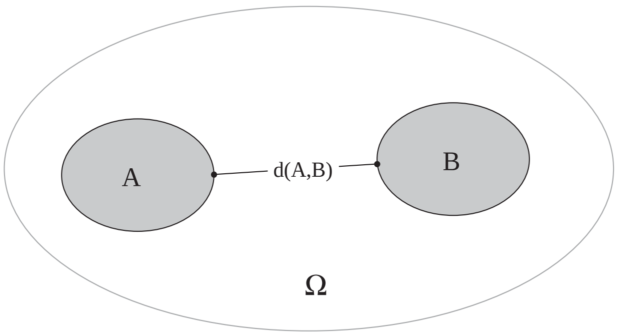

Figure 3 Sets A and B

Consider the function $u(t,x) = e^{t\Delta_\Omega}\mathbf{1}_A$. We can write

$$\begin{aligned}\int_B\int_A p_\Omega(t,x,y)d\mu(y)d\mu(x) &= \int_B\left(\int_\Omega p_\Omega(t,x,y)\mathbf{1}_A d\mu(y)\right)d\mu(x)\\ &= \int_B u(t,x)d\mu(x)\\ &\leq \mu(B)^{1/2}\left(\int_B u^2(t,x)d\mu(x)\right)^{1/2}.\end{aligned} \tag{3.6}$$

Let us set, for some $\alpha > 0$,

$$\xi(t,x) := \alpha d(x,A) - \frac{\alpha^2}{2}t$$

and consider the function

$$J(t) := \int_\Omega u^2(t,x) e^{\xi(t,x)} d\mu(x),$$

which, by Lemma (3.1) is non-increasing in $t > 0$. If $x \in B$ then

$$\xi(t,x) \geq \alpha d(B,A) - \frac{\alpha^2}{2}t,$$

whence

$$\begin{aligned} J(t) &\geq \int_B u^2(t,x) e^{\xi(t,x)} d\mu(x) \\ &\geq \exp\left(\alpha d(A,B) - \frac{\alpha^2}{2}t\right) \int_B u^2(t,x) d\mu(x). \end{aligned} \tag{3.7}$$

On the other hand, if $x \in A$ then $\xi(0,x) = 0$. By the continuity of $J(t)$ at $t = 0+$, we have

$$J(t) \leq J(0) = \int_\Omega e^{\xi(0,x)} \mathbf{1}_A d\mu(x) = \mu(A). \tag{3.8}$$

Combining (3.6), (3.7) and (3.8), we obtain

$$\int_A \int_B p_\Omega(t,x,y) d\mu(x) d\mu(y) \leq \sqrt{\mu(A)\mu(B)} \exp\left(-\frac{\alpha}{2} d(A,B) + \frac{\alpha^2}{4}t\right).$$

Setting here $\alpha = d(A,B)/t$ we finish the proof. ■

Remark 3.3 Using (3.4) instead of the monotonicity of J gives the better inequality

$$\int_A \int_B p(t,x,y) d\mu(x) d\mu(y) \leq \sqrt{\mu(A)\mu(B)} \exp\left(-\lambda_1(M)t - \frac{d^2(A,B)}{4t}\right), \tag{3.9}$$

where

$$\lambda_1(M) := \inf_{\Omega \subset\subset M} \lambda_1(\Omega). \tag{3.10}$$

It is possible to show that $\lambda_1(M)$ is the bottom of the spectrum of the operator $-\Delta_M$ in $L^2(M,\mu)$. Sometimes $\lambda_1(M)$ is called *the spectral radius* of the manifold M.

The second proof. Assume again that A and B are two compact subsets of a precompact region Ω. Fix some Lipschitz function $\psi(x)$ on Ω and consider the integral

$$\tilde{J}(t) := \int_\Omega u^2(t,x) e^{\psi(x)} d\mu(x),$$

where $u(t,x)$ solves the heat equation in $\mathbb{R}_+ \times \Omega$ and vanishes on $\partial\Omega$. Easy computation shows that

$$\tilde{J}'(t) = 2\int_\Omega u\Delta u\, e^\psi = -2\int_\Omega |\nabla u|^2 e^\psi - 2\int_\Omega u e^\psi (\nabla u, \nabla\psi).$$

Applying the inequality

$$-2u(\nabla u, \nabla\psi) \leq 2|\nabla u|^2 + \frac{1}{2}u^2 |\nabla\psi|^2,$$

we obtain

$$\tilde{J}'(t) \leq \frac{1}{2}\int_\Omega u^2 e^\psi |\nabla\psi|^2 d\mu. \tag{3.11}$$

Let us set $\psi(x) = \alpha d(x, A)$, for some $\alpha > 0$. Then $|\nabla\psi| \le \alpha$ and (3.11) implies $\tilde{J}' \le \frac{1}{2}\alpha^2 \tilde{J}$ whence

$$\tilde{J}(t) \le \tilde{J}(0) \exp(\frac{1}{2}\alpha^2 t). \tag{3.12}$$

Let us apply the above to the function $u = e^{t\Delta_\Omega}\mathbf{1}_A$. Since

$$\tilde{J}(0) = \int_\Omega \mathbf{1}_A \exp\left(\alpha d(x, A)\right) d\mu(x) = \mu(A),$$

(3.12) implies

$$\int_\Omega u^2(t, x) \exp\left(\alpha d(x, A)\right) d\mu(x) \le \mu(A) \exp(\frac{1}{2}\alpha^2 t)$$

and

$$\int_B u^2(t, x) d\mu(x) \le \mu(A) \exp\left(-\alpha d(A, B) + \frac{1}{2}\alpha^2 t\right).$$

Choosing $\alpha = d(A, B)/t$ and applying (3.6), we finish the proof. ∎

The third proof. This proof is less elementary than the previous two, but it yields the better estimate:

$$\int_A \int_B p(t, x, y) d\mu(x) d\mu(y) \le \sqrt{\mu(A)\mu(B)} \int_\delta^\infty \frac{1}{\sqrt{\pi t}} \exp\left(-\frac{s^2}{4t}\right) ds, \tag{3.13}$$

where $\delta = d(A, B)$. Indeed, it is possible to prove that

$$\int_\delta^\infty \frac{1}{\sqrt{\pi t}} \exp\left(-\frac{s^2}{4t}\right) ds \le \min(1, \frac{2}{\sqrt{\pi}} \frac{\sqrt{t}}{\delta}) \exp\left(-\frac{\delta^2}{4t}\right). \tag{3.14}$$

Therefore, (3.13) is better than (3.5) when $\delta >> \sqrt{t}$.

The inequality (3.13) is a particular case of a more general inequality of Cheeger, Gromov Taylor [27, Proposition 1.1], which says the following. Let $\phi \in L^1(\mathbb{R}_+)$ and Φ be its cos-Fourier transform, that is,

$$\Phi(\lambda) = \int_0^\infty \phi(s) \cos(s\lambda) ds. \tag{3.15}$$

The function Φ is bounded and continuous so that we can consider the bounded operator $\Phi(\sqrt{-\Delta_M})$ in $L^2(M, \mu)$ in the sense of the spectral theory. Then, for any function $f \in L^2(M, \mu)$ and any $\delta > 0$, we have

$$\left\| \Phi(\sqrt{-\Delta_M})\, f \right\|_{L^2(M \setminus \mathrm{supp}_\delta f)} \le \|f\| \int_\delta^\infty |\phi(s)|\, ds \tag{3.16}$$

where $\mathrm{supp}_\delta f$ means the δ-neighborhood of $\mathrm{supp}\, f$ and $\|\cdot\| = \|\cdot\|_{L^2(M)}$.

Given (3.16), let us take another function $g \in L^2(M, \mu)$ and suppose that the distance between the supports of f and g is at least δ. Then (3.16) yields

$$\int_M g\Phi\left(\sqrt{-\Delta_M}\right) f\, d\mu \le \|f\|\, \|g\| \int_\delta^\infty |\phi(s)|\, ds \tag{3.17}$$

(see also [32, Proposition 3.1]). Fix some $t > 0$ and take

$$\phi(s) = \frac{1}{\sqrt{\pi t}} \exp\left(-\frac{s^2}{4t}\right).$$

Then $\Phi(\lambda) = \exp\left(-t\lambda^2\right)$ and $\Phi(\sqrt{-\Delta_M}) = \exp\left(t\Delta_M\right)$ which is the heat semigroup. Hence, (3.17) implies

$$\int_M \int_M g(x) p(t, x, y) f(y) d\mu(y) d\mu(x) \le \|f\|\, \|g\| \int_\delta^\infty \frac{1}{\sqrt{\pi t}} \exp\left(-\frac{s^2}{4t}\right) ds,$$

and (3.13) follows by taking $f = \mathbf{1}_A$ and $g = \mathbf{1}_B$.

The proof of (3.16) is based on the fact that the function

$$u(t,\cdot) = \cos(t\sqrt{-\Delta_M})f$$

solves the Cauchy problem for *the wave equation*

$$\begin{cases} u_{tt} = \Delta u \\ u|_{t=0} = f \quad \text{and} \quad u_t|_{t=0} = 0. \end{cases}$$

The wave equation possesses *the finite propagation speed* equal to 1, which means that the support of the solution at time t lies in the t-neighborhood of the support of the initial data. Hence,

$$\operatorname{supp} u(t,\cdot) \subset \operatorname{supp}_t f\,. \tag{3.18}$$

Denote $w = \Phi(\sqrt{-\Delta_M})\, f$. Then, by (3.15),

$$w(x) = \int_0^\infty \phi(s)\cos(s\sqrt{-\Delta_M})f(x)ds = \int_0^\infty \phi(s)u(s,x)ds.$$

If $x \notin \operatorname{supp}_t f$ then, by (3.18), $u(s,x) = 0$ for all $s \le t$. Hence, for those x, we have

$$w(x) = \int_t^\infty \phi(s)u(s,x)ds = \int_t^\infty \phi(s)\cos(s\sqrt{-\Delta_M})f(x)ds$$

and, using $|\cos| \le 1$,

$$\begin{aligned} \|w\|_{L^2(M\setminus \operatorname{supp}_t v)} &\le \int_t^\infty \phi(s)\left\|\cos(s\sqrt{-\Delta_M})\right\|_{L^2\to L^2}\|f\|\,ds \\ &= \|f\|\int_t^\infty \phi(s)ds, \end{aligned}$$

which was to be proved. ■

Lemma 3.1 and Theorem 3.2 can be used for obtaining heat kernel upper and lower bounds, estimating the eigenvalues of the Laplace operator, obtaining conditions for stochastic completeness etc. Some of the applications are show in the next sections.

3.3 Stochastic completeness

A Riemannian manifold M is called *stochastically complete* if, for all $x \in M$ and $t > 0$,

$$\int_M p(t,x,y)d\mu(y) = 1. \tag{3.19}$$

In term of the Brownian motion X_t, (3.19) means that the total probability of X_t to be found on M is equal to 1. The opposite can happen, for example, if M is an open bounded region on $\mathbb{R}^n$ and X_t is the Brownian motion on M with the killing boundary conditions on ∂M. Indeed, the process X_t riches the boundary in finite time with positive probability and then X_t stops existing as a point in M, which makes the integral in (3.19) smaller than 1. However, Azencott [5] showed that even a geodesically complete manifold may be stochastically incomplete. On such a manifold, the Brownian particle moves away extremely fast so that it covers an infinite distance in a finite time. This happens for a geometric reason - the manifold like that has a lot of space in a neighborhood of infinity which “draws” there a Brownian particle.

The following theorem provides a test for stochastic completeness in terms of the volume growth.

Theorem 3.4 *([65]) Let M be a geodesically complete manifold. Assume that, for some point $x \in M$,*

$$\int^\infty \frac{rdr}{\log V(x,R)} = \infty, \tag{3.20}$$

where $V(x,r) = \mu(B(x,r))$. Then M is stochastically complete.

For example, (3.20) holds if $V(x,R) \leq C\exp\left(CR^2\right)$. In particular, a geodesically complete manifold with bounded below Ricci curvature is stochastically complete. This was first proved by Yau [140].

The proof of Theorem 3.4 can be found in [65] and [74]. It uses the same approach as in the proof of Lemma 3.1 but in a more sophisticated way. A reader interested in further consideration of stochastic completeness and related questions is referred to the survey [74].

4 Eigenvalues estimates

In this section we show an application of Theorem 3.2 for eigenvalue estimates. Let M be a compact connected Riemannian manifold. Denote by

$$0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq ... \leq \lambda_k \leq ...$$

the eigenvalues of $-\Delta_M$ and by $\phi_k(x)$ their corresponding eigenfunctions forming an orthonormal basis in $L^2(M)$.

Theorem 4.1 *(Chung – Grigor'yan – Yau [31]) Let M be a compact Riemannian manifold. Let A_1, A_2,...,A_k be k disjoint closed set on M. Denote*

$$\delta := \min_{i\neq j} d(A_i, A_j).$$

Then

$$\lambda_k \leq \frac{4}{\delta^2}\max_{i\neq j}\left(\log\frac{2\mu(M)}{\sqrt{\mu(A_i)\mu(A_j)}}\right)^2. \tag{4.1}$$

In particular, if we have two sets $A_1 = A$ and $A_2 = B$ then (4.1) becomes

$$\lambda_2(M) \leq \frac{4}{\delta^2}\left(\log\frac{2\mu(M)}{\sqrt{\mu(A)\mu(B)}}\right)^2, \tag{4.2}$$

where $\delta = d(A,B)$.

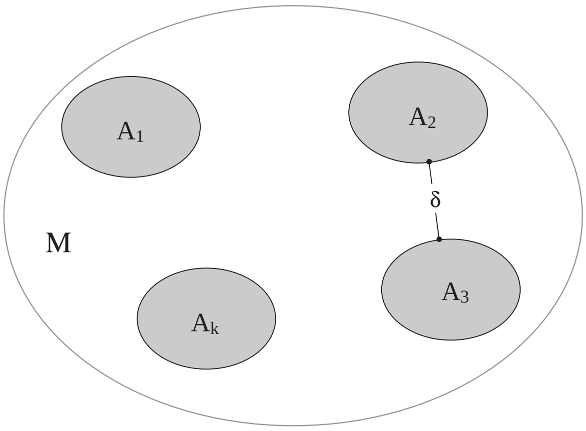

Figure 4 Sets A_i on a compact manifold M

Proof. We first prove (4.2). By the eigenfunction expansion (2.9), we can write, for any $t > 0$,

$$\int_A\int_B p(t,x,y)d\mu(x)d\mu(y) = \sum_{i=1}^{\infty} e^{-t\lambda_i}\int_A \phi_i(x)d\mu(x)\int_B \phi_i(y)d\mu(y).$$

Denote

$$a_i := \int_A \phi_i(x)d\mu(x) = (\mathbf{1}_A, \phi_i)_{L^2(M)}, \quad b_i := (\mathbf{1}_B, \phi_i)_{L^2(M)}$$

and observe that a_i and b_i are the Fourier coefficients of the functions $\mathbf{1}_A$ and $\mathbf{1}_B$ in the basis $\{\phi_i\}$, whence

$$\sum_{i=1}^{\infty} a_i^2 = \|\mathbf{1}_A\|^2_{L^2(M)} = \mu(A) \quad \text{and} \quad \sum_{i=1}^{\infty} b_i^2 = \mu(B).$$

Since $\phi_1 \equiv 1/\sqrt{\mu(M)}$ (cf. (2.14)), we obtain

$$a_1 = (\mathbf{1}_A, \frac{1}{\sqrt{\mu(M)}})_{L^2(M)} = \frac{\mu(A)}{\sqrt{\mu(M)}} \quad \text{and} \quad b_1 = \frac{\mu(B)}{\sqrt{\mu(M)}}.$$

Thus, we have

$$\begin{aligned}
\int_A \int_B p(t,x,y) d\mu(X) d\mu(y) &= a_1 b_1 + \sum_{i=2}^{\infty} e^{-t\lambda_i} a_i b_i \\
&\geq a_1 b_1 - e^{-t\lambda_2} \left(\sum_{i=2}^{\infty} a_i^2 \right)^{1/2} \left(\sum_{i=2}^{\infty} b_i^2 \right)^{1/2} \\
&\geq \frac{\mu(A)\mu(B)}{\mu(M)} - e^{-t\lambda_2} \sqrt{\mu(A)\mu(B)}.
\end{aligned}$$

Comparing with the Davies inequality (3.5), we obtain

$$\sqrt{\mu(A)\mu(B)} e^{-\frac{\delta^2}{4t}} \geq \frac{\mu(A)\mu(B)}{\mu(M)} - e^{-t\lambda_2} \sqrt{\mu(A)\mu(B)}$$

and

$$e^{-t\lambda_2} \geq \frac{\sqrt{\mu(A)\mu(B)}}{\mu(M)} - e^{-\frac{\delta^2}{4t}}$$

Choosing t so that

$$e^{-\frac{\delta^2}{4t}} = \frac{1}{2} \frac{\sqrt{\mu(A)\mu(B)}}{\mu(M)},$$

we conclude

$$\lambda_2 \leq \frac{1}{t} \log \frac{2\mu(M)}{\sqrt{\mu(A)\mu(B)}} = \frac{4}{\delta^2} \left(\log \frac{2\mu(M)}{\sqrt{\mu(A)\mu(B)}} \right)^2,$$

which is (4.2).

Let us now turn to the case $k > 2$. Consider the following integrals

$$J_{lm} := \int_{A_l} \int_{A_m} p(t,x,y) d\mu(x) d\mu(y)$$

and denote

$$a_i^{(l)} := (\mathbf{1}_{A_l}, \phi_i).$$

Then exactly as above, we have

$$\begin{aligned}
J_{lm} &= \sum_{i=1}^{\infty} a_i^{(l)} a_j^{(m)} \\
&= \frac{\mu(A_l)\mu(A_m)}{\mu(M)} + \sum_{i=2}^{k-1} e^{-\lambda_i t} a_i^{(l)} a_i^{(m)} + \sum_{i=k}^{\infty} e^{-\lambda_i t} a_i^{(l)} a_i^{(m)} \\
&\geq \frac{\mu(A_l)\mu(A_m)}{\mu(M)} + \sum_{i=2}^{k-1} e^{-\lambda_i t} a_i^{(l)} a_i^{(m)} - e^{-\lambda_k t} \sqrt{\mu(A_l)\mu(A_m)}. \qquad (4.3)
\end{aligned}$$

On the other hand, by Theorem 3.2,

$$J_{lm} \leq \sqrt{\mu(A_l)\mu(A_m)}e^{-\frac{\delta^2}{4t}}. \tag{4.4}$$

Therefore, we can further argue as in the case $k = 2$ provided the middle term in (4.3) can be discarded, that is,

$$\sum_{i=2}^{k-1} e^{-\lambda_i t} a_i^{(l)} a_i^{(m)} \geq 0. \tag{4.5}$$

Let us show that (4.5) can be achieved by *choosing* l, m. To that end, let us interpret the sequence $a^{(j)} := \left(a_2^{(j)}, a_3^{(j)}, ..., a_{k-1}^{(j)}\right)$ as a $(k-2)$-dimensional vector in $\mathbb{R}^{k-2}$. Here j ranges from 1 to k so that we have k vectors $a^{(j)}$ in $\mathbb{R}^{k-2}$. Let us introduce the inner product of vectors $u = (u_2, ..., u_{k-1})$ and $v = (v_2, ..., v_{k-1})$ in $\mathbb{R}^{k-2}$ by

$$(u, v)_t := \sum_{i=2}^{k-1} e^{-\lambda_i t} u_i v_i \tag{4.6}$$

and apply the following elementary fact:

Lemma 4.2 *From any $n+2$ vectors in n-dimensional Euclidean space, it is possible to choose two vectors with non-negative inner product.*

Note that $n+2$ is the smallest number for which the statement of Lemma 4.2 is true. Indeed, if $e_1, e_2, ..., e_n$ denote an orthonormal basis in the given space, let us set $v := -e_1 - e_2 - ... - e_n$. Then any two of the following $n + 1$ vectors

$$e_1 + \varepsilon v,\ e_2 + \varepsilon v,\ ....,\ e_n + \varepsilon v,\ v$$

have a negative inner product, provided $\varepsilon > 0$ is small enough.

Lemma 4.2 is easily proved by induction in n. The inductive step is shown on Fig. 5. Indeed, assume that the $n + 2$ vectors $v_1, v_2, ..., v_{n+2}$ form pairwise obtuse angles. Denote by E the hyperplane orthogonal to v_{n+2} and by v_i' the projection of v_i onto E. Each vector v_i with $i \leq n + 1$ can be represented as

$$v_i = v_i' - \varepsilon_i v_{n+2}$$

with $\varepsilon_i := -(v_i, v_{n+2}) > 0$. Therefore,

$$(v_i, v_j) = \left(v_i', v_j'\right) + \varepsilon_i \varepsilon_j \left|v_{n+2}\right|^2,$$

and we see that $(v_i, v_j) \geq 0$ provided $\left(v_i', v_j'\right) \geq 0$. The latter is true by the inductive hypothesis, for some i, j, whence the former holds, too.

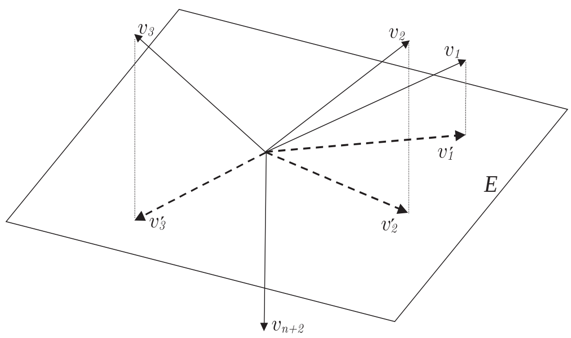

Figure 5 The vectors v_i' are projections of v_i's onto E

Let us finish the proof of Theorem 4.1. Fix some $t > 0$. By Lemma 4.2, we can find l, m so that $\left(a^{(l)}, a^{(m)}\right)_t \geq 0$ and (4.5) holds. Then (4.3) and (4.4) yield

$$e^{-t\lambda_k} \geq \frac{\sqrt{\mu(A_l)\mu(A_m)}}{\mu(M)} - e^{-\frac{\delta^2}{4t}},$$

and we are left to choose t. However, t should not depend on l, m because we use t to define the inner product (4.6) *before* choosing l, m. So, we first write

$$e^{-t\lambda_k} \geq \min_{i,j} \frac{\sqrt{\mu(A_i)\mu(A_j)}}{\mu(M)} - e^{-\frac{\delta^2}{4t}}$$

and then define t by

$$e^{-\frac{\delta^2}{4t}} = \frac{1}{2} \min_{i,j} \frac{\sqrt{\mu(A_i)\mu(A_j)}}{\mu(M)},$$

whence (4.1) follows. ∎

Somewhat sharper estimates of the eigenvalues can be obtained by using (3.13) instead of (3.5) - see [32].

5 Pointwise estimates of the heat kernel

We discuss here two methods of obtaining the Gaussian upper bounds of the heat kernel $p(t, x, y)$, that is, the estimates containing the factor $\exp\left(-\frac{d^2}{Ct}\right)$ where $d = d(x, y)$. The first approach is based on properties of weighted integrals of the heat kernel in the spirit of Lemma 3.1. The second method is based on Theorem 3.2 and on certain mean-value inequality.

5.1 Gaussian upper bounds for the heat kernel

Let M be so far an arbitrary Riemannian manifold. We start we an observation that

$$p(t, x, x) = \int_M p^2(t/2, x, z)d\mu(z) \tag{5.1}$$

which follows from the semigroup identity (2.11) and the symmetry (2.12) of the heat kernel. Using the semigroup identity again and the Cauchy–Schwarz inequality, we obtain

$$\begin{aligned} p(t, x, y) &= \int_M p(t/2, x, z)p(t/2, y, z)d\mu(z) \\ &\leq \left(\int_M p^2(t/2, x, z)d\mu(z)\right)^{\frac{1}{2}} \left(\int_M p^2(t/2, y, z)d\mu(y)\right)^{\frac{1}{2}}, \end{aligned}$$

whence, by (5.1),

$$p(t, x, y) \leq \sqrt{p(t, x, x)p(t, y, y)}. \tag{5.2}$$

For example, if we knew an *on-diagonal* estimate like

$$p(t, x, x) \leq f(t), \quad \forall x \in M,$$

it would imply the *off-diagonal* estimate

$$p(t, x, y) \leq f(t), \quad \forall x, y \in M.$$

However, the latter does not take into account the distance between x and y. To fix that, we will modify the above argument to introduce the Gaussian factor.

Let us consider the following weighted integral of the heat kernel:

$$E_D(t,x) := \int_M p^2(t,x,z) \exp\left(\frac{d^2(x,z)}{Dt}\right) d\mu(z), \tag{5.3}$$

where $D > 0$ will be specified later. In the limit case $D = \infty$, we obtain by (5.1)

$$E_\infty(t,x) = p(2t,x,x), \tag{5.4}$$

and (5.2) can be rewritten as

$$p(t,x,y) \le \sqrt{E_\infty(t/2,x)E_\infty(t/2,y)}.$$

It turns out that a similar estimate holds for a finite D.

Lemma 5.1 *([69, Proposition 5.1])We have, for any $D > 0$ and all $x, y \in M$, $t > 0$,*

$$p(t,x,y) \le \sqrt{E_D(t/2,x)E_D(t/2,y)} \exp\left(-\frac{d^2(x,y)}{2Dt}\right). \tag{5.5}$$

Proof. For any points $x, y, z \in M$, let us denote $\alpha = d(y,z)$, $\beta = d(x,z)$ and $\gamma = d(x,y)$. By the triangle inequality, $\alpha^2 + \beta^2 \ge \frac{1}{2}\gamma^2$.

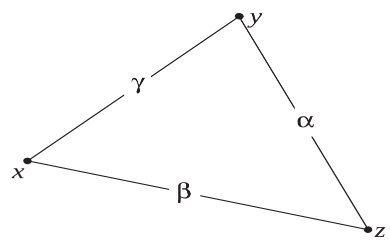

Figure 6 Distances α, β, γ

We have then

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

which was to be proved. ■

It is not a priori clear that $E_D(t,x)$ is *finite.* Indeed, it is easy to see that in $\mathbb{R}^n$, $E_D = \infty$ for all $D \le 2$. Nevertheless, the following is true.

Theorem 5.2 *([66], [69]) For any manifold M, $E_D(t,x)$ is finite for all $D > 2$, $t > 0$, $x \in M$. Moreover, $E_D(t,x)$ is non-increasing in t.*

The most non-trivial part of this theorem is the finiteness of E_D. The non-increasing of E_D is an immediate consequence of Lemma 3.1.

Furthermore, the function

$$E_D(t,x) \exp(2\lambda_1(M)t)$$

is also non-increasing in t, which follows from (3.4) (recall that the spectral radius $\lambda_1(M)$ is defined by (3.10)). Inequality (5.5) implies, for all $t_0 > 0$ and $t > 0$,

$$p(t,x,y) \le \sqrt{E_D(\tau/2,x)E_D(\tau/2,y)}e^{\lambda_1(M)t_0}\exp\left(-\lambda_1(M)t - \frac{d^2(x,y)}{2Dt}\right), \tag{5.6}$$

where $\tau = \min(t,t_0)$. Indeed, if $t \ge t_0$ then (5.6) follows from (5.5) and

$$E_D\left(t/2,x\right)\exp\left(\lambda_1(M)t\right) \le E_D(t_0/2)\exp\left(\lambda_1(M)t_0\right). \tag{5.7}$$

If $t < t_0$ then (5.6) follows from (5.5) directly.

If $\lambda_1(M) > 0$ then (5.6) provides already a good upper bound of the heat kernel which can be rewritten as follows, for $t > t_0$,

$$p(t,x,y) \le \Phi(x,y)\exp\left(-\lambda_1(M)t - \frac{d^2(x,y)}{2Dt}\right), \tag{5.8}$$

where

$$\Phi(x,y) := \sqrt{E_D(t_0/2,x)E_D(t_0/2,y)}e^{\lambda_1(M)t_0}.$$

However, if $\lambda_1(M) = 0$ then (5.6) is of no use and, by Lemma 5.1, the question of obtaining the long time behaviour of $p(t,x,y)$ amounts to the same question for $E_D(t,x)$. The latter is reduced by the following theorem to the *on-diagonal* rate of decay of $p(t,x,x)$ in t.

Theorem 5.3 *(Ushakov [129], Grigor'yan [72]) Assume that, for some $x \in M$ and for all $t > 0$,*

$$p(t,x,x) \le \frac{C}{f(t)}, \tag{5.9}$$

*where $f(t)$ is an increasing positive function on $(0,+\infty)$ satisfying certain regularity condition (*see below*). Then, for all $D > 2$ and $t > 0$,*

$$E_D(t,x) \le \frac{C'}{f(\varepsilon t)}, \tag{5.10}$$

for some $\varepsilon > 0$ and C'.

Remark 5.4 If (5.9) holds for $t \le t_0$ then (5.10) also holds for $t \le t_0$. Indeed, extend the function $f(t)$ by the constant $f(t_0)$ for $t > t_0$. Then (5.9) is true for all t because $p(t,x,x)$ is non-increasing in t as was remarked at the end of Section 3.1. Hence, by Theorem 5.3, (5.10) is true, too.

The regularity condition is the following: there are numbers $A \ge 1$ and $a > 1$ such that

$$\frac{f(as)}{f(s)} \le A\frac{f(at)}{f(t)}, \quad \text{for all } 0 < s < t. \tag{5.11}$$

The constants ε and C' in the statement of Theorem 5.3 depend on A and a. There are two simple situations when (5.11) holds:

1. $f(t)$ satisfies *the doubling condition,* that is, for some $A > 1$,

$$f(2t) \le Af(t), \quad \forall t > 0. \tag{5.12}$$

Then (5.11) holds with $a = 2$ because

$$\frac{f(2s)}{f(s)} \le A \le A\frac{f(2t)}{f(t)}.$$

2. $f(t)$ has *at least polynomial growth* in the sense that, for some $a > 1$, the function $f(at)/f(t)$ is increasing in t. Then (5.11) holds for $A = 1$.

If f is differentiable then (5.11) is implied by either of the following properties of the function $l(\xi) := \log f(e^{\xi})$ defined in $(-\infty, +\infty)$:

1. l' *is uniformly bounded* (for example, this is the case when $f(t) = t^N$ or $f(t) = \log^N(1+t)$ where $N > 0$);

2. l' *is monotone increasing* (for example, $f(t) = \exp(t^N)$).

On the other hand, (5.11) fails if $l' = \exp(-\xi)$ (it is unbounded as $\xi \to -\infty$) which corresponds to $f(t) = \exp\left(-t^{-1}\right)$. Also, (5.11) may fail if l' is oscillating.

By putting together Theorem 5.3 and Lemma 5.1, we obtain

Corollary 5.5 *Assume that, for some points $x, y \in M$ and for all $t > 0$,*

$$p(t,x,x) \le \frac{C}{f(t)} \quad \text{and} \quad p(t,y,y) \le \frac{C}{g(t)}, \tag{5.13}$$

where f and g are increasing positive function on $(0, +\infty)$ satisfying the regularity condition (5.11) as above. Then, for all $t > 0$, $D > 2$ and for some $\varepsilon > 0$

$$p(t,x,y) \le \frac{C'}{\sqrt{f(\varepsilon t) g(\varepsilon t)}} \exp\left(-\frac{d^2(x,y)}{2Dt}\right). \tag{5.14}$$

Remark 5.6 By using (5.6) instead of (5.5) we obtain, for all $t_0 > 0$,

$$p(t,x,y) \le \frac{C' e^{\lambda_1(M) t_0}}{\sqrt{f(\varepsilon \tau) g(\varepsilon \tau)}} \exp\left(-\lambda_1(M) t - \frac{d^2(x,y)}{2Dt}\right), \tag{5.15}$$

where $\tau = \min(t, t_0)$. Note that (5.13) may be assumed only for $t \le t_0$. One can always extend $f(t)$ and $g(t)$ for $t > t_0$ by the constants $f(t_0)$ and $g(t_0)$, respectively, and (5.13) will continue to be true by the non-increasing of $p(t,x,x)$ in t.

Hence, the question of obtaining the Gaussian upper bounds of the heat kernel is reduced to obtaining the on-diagonal estimates (5.13), which will be considered in Section 6.

For the proof of Theorem 5.3, the reader is referred to [72]. The proof uses the integral maximum principle of Lemma 3.1. Note that if f and g satisfy the doubling property (5.12) then ε in (5.14) and (5.15) can be absorbed into the constant C'.

The finiteness of $E_D(t,x)$ in Theorem 5.2 can be deduced from Theorem 5.3. All that one needs is the initial upper bound $p(t,x,x) \le C_x t^{-n/2}$, for small t, which can be obtained by Theorem 5.8 from the next Section. See [66] or [69] for details.

Historically, the first method of obtaining the Gaussian upper bounds for the heat kernel of a uniformly elliptic operators in $\mathbb{R}^n$ with variable coefficients was introduced by Aronson [4]. He used the integral maximum principle but in a different way. The estimates of Aronson use the Euclidean distance rather than the Riemannian distance associated with the coefficients. Varadhan [130], [131] first realized that the Riemannian distance should be used instead. His result implies that, on any manifold,

$$\lim_{t \to 0+} t \log p(t,x,y) = -\frac{1}{4} d^2(x,y).$$

The first uniform Gaussian estimates for the heat kernel on manifolds was obtained by Cheng, Li and Yau [29], for manifolds of bounded geometry (see Section 7 below). They were later improved by Cheeger, Gromov and Taylor [27] by using (3.16). The sharp heat kernel estimates for the manifolds of non-negative Ricci curvature was obtained by Li and Yau [98]. Further progress in Gaussian upper bounds (under non-curvature assumptions) is due to Davies [41], [42], [43]. See also [135]. The approach to the Gaussian bounds we have adopted here is due to the author [69], [72].

5.2 Mean-value property

Here we present an alternative method of obtaining Gaussian upper bounds like (5.14), which avoids using $E_D(t,x)$ and, instead, is based on Theorem 3.2 and on the mean-value property. This method was introduced by Davies [45]. The treatment of this section is close to that in [97] and [37].

Fix some distinct points $x, y \in M$ and consider the balls $B(x,r)$, $B(y,r)$. By Theorem 3.2, we have

$$\int_{B(x,r)} \int_{B(y,r)} p(t,\xi,\eta) d\mu(\eta) d\mu(\xi) \leq \sqrt{V(x,r)V(y,r)} \exp\left(-\frac{(d-2r)_+^2}{4t}\right), \tag{5.16}$$

where $V(x,r) := \mu(B(x,r))$ and $d = d(x,y)$. If we knew that the value of the heat kernel at (t,x,y) can be estimated via the integral in (5.16) then we could obtain from (5.16) an upper bound for $p(t,x,y)$. This can be done by using the following *mean-value property.*

Definition 5.7 *We say that the manifold M admits the mean-value property (MV) if, for all $t > \tau > 0$, $\xi \in M$ and for any positive solution $u(s,\eta)$ of the heat equation in the cylinder $(t-\tau, t] \times B(\xi, \sqrt{\tau})$, we have*

$$u(t,\xi) \leq \frac{C}{\tau V(\xi,\sqrt{\tau})} \int_{t-\tau}^{t} \int_{B(\xi,\sqrt{\tau})} u(s,\eta) d\mu(\eta) ds. \tag{5.17}$$

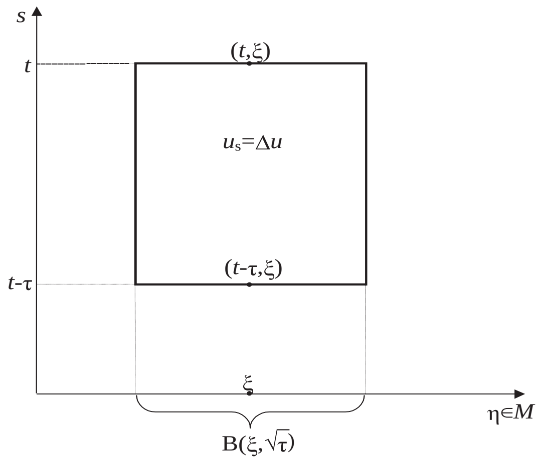

Figure 7 Cylinder $(t-\tau, t) \times B(\xi, \sqrt{\tau})$

The geometric assumptions which imply (MV), will be discussed in Section 6.4. Here we only mention that (5.17) holds, for example, if M is a geodesically complete manifold of nonnegative Ricci curvature.

Theorem 5.8 *(Li – Wang [97], Coulhon – Grigor'yan [37]) Assume that the mean-value property (MV) holds on the manifold M. Then, for all $x \in M$ and $t > 0$,*

$$p(t,x,x) \leq \frac{C}{V(x,\sqrt{t})}. \tag{5.18}$$

Moreover, for all $x, y \in M$, $t > 0$, $D > 2$,

$$p(t,x,y) \leq \frac{C'}{\sqrt{V(x,\sqrt{t/2})V(y,\sqrt{t/2})}} \exp\left(-\frac{d^2(x,y)}{2Dt}\right). \tag{5.19}$$

Hence, (5.19) holds on complete manifolds of non-negative Ricci curvature. For those manifolds, this estimate was first proved by different method by Li and Yau [98]. Moreover, they proved also a matching lower bound for the heat kernel which shows that (5.19) is sharp up to the values of the constants (see Sections 5.3 and 7.8 for the lower bounds of the heat kernel). In $\mathbb{R}^n$, we have $V(x, \sqrt{t}) \asymp t^{n/2}$ so that (5.18) and (5.19) give the correct rate for the long time decay of the heat kernel.

Proof of Theorem 5.8. Let us start with the consequence of (2.19)

$$\int_M p(s,x,z)d\mu(z) \leq 1 \tag{5.20}$$

and integrate it in time s:

$$\int_0^t \int_M p(s,x,z)d\mu(z) \leq t.$$

Applying (5.17) for $u = p(\cdot, x, \cdot)$, we obtain

$$p(t,x,x) \leq \frac{C}{tV(x,\sqrt{t})} \int_0^t \int_{B(x,\sqrt{t})} p(s,x,z)d\mu(z) \leq \frac{C}{V(x,\sqrt{t})},$$

which is exactly (5.18).

To show (5.19), we argue similarly but use (5.16) instead of (5.20). We start with (5.17) applied to the function $u = p(\cdot, \cdot, y)$,

$$p(t,x,y) \leq \frac{C}{\tau V(x,\sqrt{\tau})} \int_{t-\tau}^{t} \int_{B(x,\sqrt{\tau})} p(s,\xi,y)d\mu(\xi)ds, \tag{5.21}$$

for some $\tau \in (0,t)$. On the other hand, also by (5.17) applied to the function $u = p(\cdot, \xi, \cdot)$,

$$p(s,\xi,y) \leq \frac{C}{\tau V(y,\sqrt{\tau})} \int_{s-\tau}^{s} \int_{B(y,\sqrt{\tau})} p(\theta,\xi,\eta)d\mu(\eta)d\theta. \tag{5.22}$$

Combining (5.21) and (5.22), we see that $p(t,x,y)$ is bounded above by

$$\begin{aligned}
&\frac{C^2}{\tau^2 V(x,\sqrt{\tau})V(y,\sqrt{\tau})} \int_{t-\tau}^{t}\int_{s-\tau}^{s}\int_{B(x,\sqrt{\tau})}\int_{B(y,\sqrt{\tau})} p(\theta,\xi,\eta)d\mu(\eta)d\mu(\xi)d\theta ds \\
\leq\;& \frac{C^2}{\tau V(x,\sqrt{\tau})V(y,\sqrt{\tau})} \int_{t-2\tau}^{t}\int_{B(x,\sqrt{\tau})}\int_{B(y,\sqrt{\tau})} p(\theta,\xi,\eta)d\mu(\eta)d\mu(\xi)d\theta\,,
\end{aligned}$$

where we have assumed $\tau \leq t/2$. Using (5.16), we obtain

$$\begin{aligned}
p(t,x,y) &\leq \frac{C^2}{\tau\sqrt{V(x,\sqrt{\tau})V(y,\sqrt{\tau})}} \int_{t-2\tau}^{t} \exp\left(-\frac{(d-2\sqrt{\tau})_+^2}{4\theta}\right)d\theta \\
&\leq \frac{2C^2}{\sqrt{V(x,\sqrt{\tau})V(y,\sqrt{\tau})}} \exp\left(-\frac{(d-2\sqrt{\tau})_+^2}{4t}\right).
\end{aligned} \tag{5.23}$$

Choose $\tau = t/2$ (which is the maximal τ we can take). If $d \geq C\sqrt{t}$ where C is large enough then

$$\frac{(d-2\sqrt{\tau})_+^2}{4t} \geq \left(1 - o(C^{-1})\right)\frac{d^2}{4t},$$

and (5.23) implies (5.19). If $d \leq C\sqrt{t}$ then the Gaussian term in (5.19) is of the order 1, and (5.19) follows again from (5.23) by discarding the Gaussian term in (5.23). ■

Theorem 5.8 admits a localized version. We say that the manifold M admits a *restricted* mean-value property (MV$xy\tau_0$), for some $x, y \in M$ and $\tau_0 \in \mathbb{R}_+$, if the inequality (5.17) holds for all $\tau \in (0, \tau_0]$ and for $\xi = x$ and $\xi = y$. If M admits (MV$xy\tau_0$) then a slight modification of the above proof yields the estimate

$$p(t,x,y) \leq \frac{C'}{\sqrt{V(x,\sqrt{\tau})V(y,\sqrt{\tau})}} \exp\left(-\lambda_1(M)t - \frac{d^2(x,y)}{2Dt}\right) \tag{5.24}$$

where $\tau = \min(t/2, \tau_0)$. The term $\lambda_1(M)t$ appears if one applies (3.9) instead of (3.5) and uses the boundedness of τ.

Observe that the property (MV$xy\tau_0$) holds on *any* manifold. Namely, for any given $x, y \in M$, there exists τ_0 such that (MV$xy\tau_0$) is true (which provides another proof of (5.8)). However, the constant C in the mean-value inequality (5.17) depends on the certain geometric properties of the balls $B(x, \sqrt{\tau_0})$ and $B(y, \sqrt{\tau_0})$.

If the volume function $V(x,\cdot)$ satisfies the doubling condition (5.12) then (5.19) follows also from (5.18), by Theorem 5.3. In this case, $\sqrt{t/2}$ in (5.19) can be replaced by $\sqrt{t}$. It is not known whether there exists a manifold with (MV) for which $V(x,\cdot)$ is not doubling. Assuming the volume doubling property, one can improve the estimate (5.19) of Theorem 5.8 as follows.

Theorem 5.9 *Assume that the mean-value property (MV) holds on the manifold M and, for all $r' \geq r$ and $x \in M$,*

$$\frac{V(x,r')}{V(x,r)} \leq C\left(\frac{r'}{r}\right)^N, \tag{5.25}$$

with some $N > 0$. Then, for all $x, y \in M$ and $t > 0$,

$$p(t,x,y) \leq \frac{C'}{\sqrt{V(x,\sqrt{t})V(y,\sqrt{t})}} \left(1 + \frac{d}{\sqrt{t}}\right)^{N-1} \exp\left(-\frac{d^2}{4t}\right) \tag{5.26}$$

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

Remark 5.10 Although (5.25) looks stronger than the doubling property for $V(x,\cdot)$, these two properties are, in fact, equivalent. However, we have preferred (5.25) because the exponent N enters the estimate (5.26) in the sharp way. Indeed, as was shown by Molchanov [105], if M is the sphere $\mathbb{S}^n$ and x and y are conjugate points on $\mathbb{S}^n$ then

$$p(t,x,y) \sim \frac{c}{t^{n/2}} \left(\frac{d}{\sqrt{t}}\right)^{n-1} \exp\left(-\frac{d^2}{4t}\right), \quad t \to 0.$$

Hence, the exponent $N-1$ in the polynomial correction term in (5.26) is sharp. See [51] for further results containing the polynomial correction term.

Proof. If $d^2 < 4t$ then (5.26) follows from (5.19). Assume now $d^2 \geq 4t$ and follow the argument of the previous proof. However, let us use (3.13) and (3.14) instead of (3.5). Then, instead of (5.23), we obtain

$$p(t,x,y) \leq \frac{4C^2}{\sqrt{V(x,\sqrt{\tau})V(y,\sqrt{\tau})}} \frac{\sqrt{t}}{(d-2\sqrt{\tau})_+} \exp\left(-\frac{(d-2\sqrt{\tau})_+^2}{4t}\right), \tag{5.27}$$

for any $\tau \leq t/2$. Let us choose $\tau = \frac{t^2}{d^2}$ which smaller than $t/2$, by $d^2 > 2t$. Then we have

$$\frac{(d-2\sqrt{\tau})^2}{4t} \geq \frac{d^2}{4t} - \frac{d\sqrt{\tau}}{t} = \frac{d^2}{4t} - 1.$$

Also, $d - 2\sqrt{\tau} = d - 2\frac{t}{d} \geq \frac{1}{2}d$, whence

$$\frac{\sqrt{t}}{d - 2\sqrt{\tau}} \leq \frac{2\sqrt{t}}{d}.$$

Finally, by (5.25),

$$V\left(x, \sqrt{\tau}\right) = V(x, \sqrt{t}\frac{\sqrt{t}}{d}) \geq C^{-1} V(x, \sqrt{t}) \left(\frac{\sqrt{t}}{d}\right)^N.$$

After substituting all these inequalities into (5.27), we obtain (5.26). ■

For other application of the mean-value property see [95], [94], [96], [97].

5.3 On-diagonal lower bounds and the volume growth

Here we show how to apply Theorem 5.2 to obtain on-diagonal lower bounds of the heat kernel.

Theorem 5.11 *(Coulhon – Grigor'yan [36]) Let M be a geodesically complete Riemannian manifold. Assume that, for some point $x \in M$ and all $r > r_0$,*

$$V(x, r) \leq C r^N, \tag{5.28}$$

with some positive constants C and N. Then, for all $t > t_0$,

$$p(t, x, x) \geq \frac{1/4}{V(x, K\sqrt{t \log t})}, \tag{5.29}$$

where $K > 0$ depend on x, r_0, C, N and $t_0 := \max(r_0^2, e)$.

Proof. Take some $\rho > 0$ and denote $\Omega = B(x, \rho)$. By the semigroup identity, we have

$$\begin{aligned} p(2t, x, x) &= \int_M p^2(t, x, y) d\mu(y) \\ &\geq \int_\Omega p^2(t, x, y) d\mu(y) \\ &\geq \frac{1}{\mu(\Omega)} \left(\int_\Omega p(t, x, y) d\mu(y)\right)^2 \\ &= \frac{1}{\mu(\Omega)} \left(1 - \int_{M \setminus \Omega} p(t, x, y) d\mu(y)\right)^2. \end{aligned} \tag{5.30}$$

In the last line, we have used the stochastic completeness of M, that is,

$$\int_M p(t, x, y) d\mu(y) = 1.$$

By Theorem 3.4, this follows from the geodesic completeness of M and from the volume growth hypothesis (5.28).

Next we will choose $\rho = \rho(t)$ so that

$$\int_{M \setminus B(x, \rho)} p(t, x, y) d\mu(y) \leq \frac{1}{2}. \tag{5.31}$$

Assume for the moment that (5.31) holds. Then (5.30) yields

$$p(2t, x, x) \geq \frac{1/4}{V(x, \rho(t))}.$$

To match (5.29), we need to estimate $\rho(t)$ as follows

$$\rho(t) \leq \text{const}\sqrt{t\log t}. \tag{5.32}$$

Let us prove (5.31) with $\rho(t)$ satisfying (5.32). We apply again the Cauchy–Schwarz inequality as follows, denoting $d = d(x,y)$ and taking some $D > 2$,

$$\begin{aligned}\left[\int_{M\setminus B(x,\rho)} p(t,x,y)d\mu(y)\right]^2 &\leq \int_M p^2(t,x,y)\exp\left(\frac{d^2}{Dt}\right)\int_{M\setminus B(x,\rho)}\exp\left(-\frac{d^2}{Dt}\right)\\ &= E_D(t,x)\int_{M\setminus B(x,\rho)}\exp\left(-\frac{d^2}{Dt}\right)d\mu(y),\end{aligned} \tag{5.33}$$

where $E_D(t,x)$ is defined by (5.3). By Theorem 5.2, we have, for all $t > t_0$,

$$E_D(t,x) \leq E_D(t_0,x) < \infty. \tag{5.34}$$

Since x is fixed, we can consider $E_D(t_0,x)$ as a constant. Let us now estimate the integral in (5.33) assuming that $\rho = \rho(t) > r_0$. By splitting the integral over the complement of $B(x,\rho)$ into the sum of the integrals over the annuli $B(x,2^{k+1}\rho)\setminus B(x,2^k\rho)$, $k = 0,1,2,...$, and using the hypothesis (5.28), we obtain

$$\int_{M\setminus B(x,\rho)}\exp\left(-\frac{d(x,y)^2}{Dt}\right)d\mu(y) \leq \sum_{k=0}^{\infty}\exp\left(-\frac{4^k\rho^2}{Dt}\right)V(x,2^{k+1}\rho) \tag{5.35}$$

$$\leq C2^N\rho^N\sum_{k=0}^{\infty}2^{Nk}\exp\left(-\frac{4^k\rho^2}{Dt}\right). \tag{5.36}$$

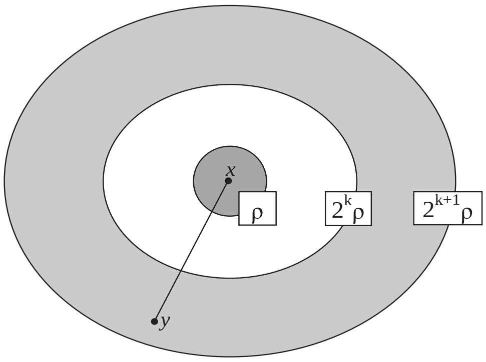

Figure 8 Annulus $B(x,2^{k+1}\rho)\setminus B(x,2^k\rho)$

Assuming $\rho^2/t \geq 1$, the sum in the line above is majorized by a geometric series whence

$$\int_{M\setminus B(x,\rho)}\exp\left(-\frac{d(x,y)^2}{Dt}\right)d\mu(y) \leq C'\rho^N\exp\left(-\frac{\rho^2}{Dt}\right). \tag{5.37}$$

By setting $\rho(t) = K\sqrt{t\log t}$ with K large enough, we make the integral above arbitrarily small, whence (5.31) follows by (5.33) and (5.34). To finish the proof, we have to make sure that $\rho(t) > r_0$. Indeed, this follows from $t > t_0 = \max(r_0^2, e)$ and $K > 1$. ■

One may wonder what is geometric background of the quantity $E_D(t_0,x)$ which we have interpreted as a constant. In fact, an upper bound of it can be proved in terms of an intrinsic geometric property of the ball $B(x,\varepsilon)$, for arbitrarily small ε - see [66] (this can be extracted also from Theorems 5.3 and 6.7). The geometric property in question is a Sobolev inequality in $B(x,\varepsilon)$ which holds because the geometry of $B(x,\varepsilon)$ is nearly Euclidean. In particular, the constant K does not depend on x if the manifold M has bounded geometry (see Section 7.5).

Note that no off-diagonal lower bound of the heat kernel can be proved under such a mild assumption as (5.28). Indeed, the manifold M may consist of two large parts connected by a thin tube. Suppose that x belongs to one part and y - to another.

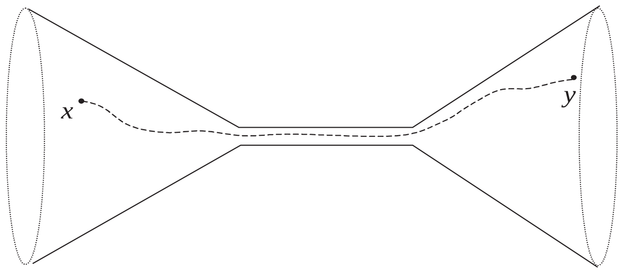

Figure 9 Manifold with a bottleneck

Then by making the tube thinner, one can get $p(t,x,y)$ to be arbitrarily small, without violating the volume growth (5.28). It is especially clear from the probabilistic point of view since the probability of the Brownian motion X_t getting from x to y can be arbitrarily small when the tube shrinks. Hence, the situation with off-diagonal lower bounds for the heat kernel is entirely different than that of upper bounds. As we have seen in Section 5.1, an on-diagonal upper bound of the heat kernel implies a Gaussian off-diagonal upper bound (see, for example, Corollary 5.5). On the contrary, the on-diagonal lower bound of the heat kernel in general does not imply anything about the off-diagonal values of the heat kernel.

Comparing the lower bound (5.29) with the upper bounds (5.18) and (5.19) (which hold, for example, on non-negatively curved manifolds) we see that both are governed by the volume of balls but with different radii[1]. Indeed, the former radius is of the order $\sqrt{t\log t}$ whereas the later is of the order $\sqrt{t}$. The radius $\sqrt{t}$ matches the heat kernel behaviour in $\mathbb{R}^n$ where we have

$$p(t,x,x)=\frac{1}{(4\pi t)^{n/2}}=\frac{\mathrm{const}}{V(x,\sqrt{t})}.$$

There is an example [36] showing that in the lower bound (5.29), one cannot in general get rid of $\log t$ assuming only the hypotheses of Theorem 5.11. However, under certain additional hypotheses, it is possible as is shown by the following statement (cf. Theorem 5.8).

Theorem 5.12 *(Coulhon – Grigor'yan [36]) Let M be a geodesically complete Riemannian manifold. Assume that, for some point $x\in M$ and all $r>0$*

$$V(x,2r)\le CV(x,r) \tag{5.38}$$

and, for all $t>0$,

$$p(t,x,x)\le\frac{C}{V(x,\sqrt{t})}. \tag{5.39}$$

Then, for all $t>0$,

$$p(t,x,x)\ge\frac{c}{V(x,\sqrt{t})}, \tag{5.40}$$

where $c>0$ depends on C.

Proof. The proof follows almost the same line as the proof of Theorem 5.11. The difference comes when estimating $E_D(t,x)$. Instead of using the monotonicity of $E_D(t,x)$, we apply Theorem 5.3. Indeed, by Theorem 5.3, the hypotheses (5.39) and (5.38) yield

$$E_D(t,x)\le\frac{C'}{V(x,\sqrt{t})}.$$

[1] The function $\rho(t)$ satisfying (5.31) is closely related to the escape rate of the Brownian motion - see [75], [73] and [76].

By substituting this into (5.33) and applying the doubling property (5.38) to estimate the sum in (5.35), we obtain instead of (5.37)

$$\int\limits_{M\setminus B(x,\rho)} \exp\left(-\frac{d(x,y)^2}{Dt}\right) d\mu(y) \le C'' \exp\left(-\frac{\rho^2}{Dt}\right). \tag{5.41}$$

Hence, the integral in (5.41) can be made arbitrarily small by choosing $\rho = K\sqrt{t}$ with K large enough.

Finally, one uses again the doubling property to write

$$p(2t,x,x) \ge \frac{1/4}{V(x,\rho(t))} \ge \frac{c}{V(x,\sqrt{2t})},$$

finishing the proof. ■

Theorem 5.11 can be extended to a more general volume growth assumption as follows.

Theorem 5.13 *([36, Theorem 6.1]) Let M be a geodesically complete Riemannian manifold. Assume that, for some point $x \in M$ and all $r > r_0$,*

$$V(x,r) \le \mathcal{V}(r),$$

where $\mathcal{V}(r) > 2$ is a continuous increasing function on (r_0,∞) such that $\frac{r^2}{\log \mathcal{V}(r)}$ is strictly decreasing in r. Define the function $\rho(t)$ by

$$t = \frac{\rho^2(t)}{\log \mathcal{V}(\rho(t))},$$

for $t > t_0 = t_0(r_0)$. Then, for all $t > t_0$,

$$p(t,x,x) \ge \frac{1/4}{V(x,\rho(Kt))},$$

where $K > 1$ depends on x and r_0.

For example, of $\mathcal{V}(r) = \exp(r^\alpha)$, $0 < \alpha < 2$, then we obtain $\rho(t) \asymp t^{\frac{1}{2-\alpha}}$ and

$$p(t,x,x) \ge c \exp\left(-Ct^{\frac{\alpha}{2-\alpha}}\right). \tag{5.42}$$

As we will see in Section 7.7, if $\alpha \le 1$ then the exponent $\frac{\alpha}{2-\alpha}$ in (5.42) is sharp - cf. (7.56).

However, (5.42) is not sharp if $\alpha > 1$, that is, if $V(x,r)$ grows superexponentially in r. Indeed, $p(t,x,x)$ cannot decay faster than exponentially in t as is said by the following statement.

Proposition 5.14 *For any manifold M, for any $x \in M$ and $\varepsilon > 0$, there exists $c = c_x > 0$ such that*

$$p(t,x,x) \ge c_x \exp\left(-\left(\lambda_1(M)+\varepsilon\right)t\right), \quad \forall t > 0, \tag{5.43}$$

where $\lambda_1(M)$ is the spectral radius defined by (3.10).

Proof. Take a precompact region Ω containing x and such that

$$\lambda_1(\Omega) \le \lambda_1(M) + \varepsilon.$$

We have $p(t,x,x) \ge p_\Omega(t,x,x)$ and, by the eigenfunction expansion (2.9),

$$p_\Omega(t,x,x) = \sum_{k=1}^{\infty} e^{-\lambda_k(\Omega)t}\phi_k^2(x) \ge e^{-\lambda_1(\Omega)t}\phi_1^2(x),$$

whence (5.43) follows. ■

Combining Proposition 5.14 with the upper bound (5.8), we obtain

Corollary 5.15 *(Li [93]) For any manifold M and for all $x \in M$,*

$$\lim_{t\to\infty} \frac{\log p(t,x,x)}{t} = -\lambda_1(M).$$

6 On-diagonal upper bounds and Faber-Krahn inequalities

In this section, we discuss mainly on-diagonal upper bounds of the heat kernel of the type

$$p(t,x,x) \le \frac{C}{f(t)}. \tag{6.1}$$

As we know from Section 5.1, the on-diagonal upper bound implies the off-diagonal Gaussian upper bound (5.14). The main emphasis will be made on geometric background of the estimate (6.1). We will consider two situations when the estimate (6.1) is well understood:

1. a uniform estimate when (6.1) is meant to hold for all $t > 0$ and $x \in M$ with *the same* function f;
2. a "relative" estimate when the function $f(t)$ depends on x as follows: $f(t) = V(x,\sqrt{t})$ (cf. (5.18)).

6.1 Polynomial decay of the heat kernel

Here we describe in the historical order the results related to the heat kernel upper bound

$$p(t,x,x) \le \frac{C}{t^{n/2}}, \quad \forall x \in M,\ t > 0, \tag{6.2}$$

which is obviously motivated by the heat kernel in $\mathbb{R}^n$. One may ask under what geometric assumptions (6.2) holds? Historically the first result was obtained by Nash [109] who discovered a simple method of deducing (6.2) from the Sobolev inequality. The latter is the following assertion

for any $f \in C_0^\infty(M)$, $f \ge 0$,

$$\left(\int_M f^{\frac{2n}{n-2}} d\mu\right)^{\frac{n-2}{n}} \le C \int_M |\nabla f|^2 \, d\mu \tag{6.3}$$

(of course, we assume $n > 2$ here).

It is well known that the Sobolev inequality (6.3) holds in $\mathbb{R}^n$. However, for a general manifold, it may not be true. In fact, the Sobolev inequality is quite sensitive to the geometry of the manifold and can be regarded itself as a geometric condition. It can be deduced from the following isoperimetric inequality: for all precompact regions Ω with smooth boundary

$$\sigma(\partial\Omega) \ge c\mu(\Omega)^{\frac{n-1}{n}} \tag{6.4}$$

(see [61] and [101]). The inequality (6.4) is well-known in $\mathbb{R}^n$. It is an obvious consequence of the isoperimetric property of a ball in $\mathbb{R}^n$: any region of the same volume as the ball has larger boundary area unless it is the ball. We will discuss the isoperimetric type inequalities in more details in Section 7.

Following Nash's argument, let us prove the following Theorem.

Theorem 6.1 *If the Sobolev inequality (6.3) is true on M then (6.2) holds, too.*

Proof. By the exhaustion argument, it suffices to prove (6.2) for p_Ω where Ω is a precompact open subset of M with smooth boundary. Fix $y \in \Omega$ and denote $u(t,x) = p(t,x,y)$ and

$$J(t) := \int_\Omega u^2(t,x) d\mu(x).$$

Arguing as in Section 3.1, we obtain

$$J'(t) = 2\int u\, u_t \, d\mu = 2\int u\Delta u \, d\mu = -2\int |\nabla u|^2 \, d\mu. \tag{6.5}$$

As in Section 3.1, we can conclude from (6.5) that $J(t)$ is non-increasing. However, we can go further by estimating the right hand side of (6.5) by using (6.3). Indeed, it is easy to see that the Sobolev inequality extends to functions like $u(\cdot,t)$ vanishing on $\partial\Omega$ whence

$$\int |\nabla u|^2 \, d\mu \geq c \left(\int u^{\frac{2n}{n-2}} d\mu \right)^{\frac{n-2}{n}}. \tag{6.6}$$

We would like to have on the right hand side of (6.6) $\int u^2$ in order to be able to create a differential inequality for $J(t)$. To that ends, we use the Hölder interpolation inequality

$$\left(\int u^\alpha d\mu \right)^{\frac{1}{\alpha-1}} \left(\int u d\mu \right)^{\frac{\alpha-2}{\alpha-1}} \geq \int u^2 d\mu, \tag{6.7}$$

which is true for all $\alpha > 2$. Naturally, we take here $\alpha = \frac{2n}{n-2}$ and obtain from (6.6) *the Nash inequality*

$$\int |\nabla u|^2 \, d\mu \geq c \left(\int u^2 d\mu \right)^{\frac{n+2}{n}} \left(\int u d\mu \right)^{-\frac{4}{n}}. \tag{6.8}$$

Observing that

$$\int u(t,x) d\mu(x) = \int p_\Omega(t,x,y) d\mu(x) \leq 1,$$

we deduce from (6.5) and (6.8) the differential inequality

$$J' \leq -cJ^{\frac{n+2}{n}}.$$

By integrating it from 0 to t, we find $J(t) \leq Ct^{-n/2}$. We are left to observe that by the semigroup property $J(t) = p_\Omega(2t,y,y)$, whence (6.2) follows. ■

In 1967, Aronson [4] proved his famous two-sided Gaussian estimates for the heat kernel associated with a uniformly elliptic operator in $\mathbb{R}^n$ (see also [116], [60], [124]). In our notation, the Aronson upper bound can be written in the form

$$p(t,x,y) \leq \frac{C}{t^{n/2}} \exp\left(-\frac{d^2(x,y)}{Ct} \right), \tag{6.9}$$

assuming that manifold M is $\mathbb{R}^n$ equipped with a Riemannian metric that is quasi-isometric to the Euclidean one. Now we know that (6.9) follows from (6.2) by Theorem 5.3. The proof of Aronson was different and used the integral maximum principle (see Lemma 3.1). Some versions of his proof can be found in [116], [66], [69].

In 1985, Varopoulos [133] proved that the Sobolev inequality is not only sufficient but also necessary for the on-diagonal upper bound (6.2). Another proof of that will follow from the results of Section 6.2 (cf. Theorem 6.5).

Two years later, Carlen, Kusuoka and Stroock [19] proved that (6.2) is also equivalent to the Nash inequality (6.8). They were also able to localize the heat kernel estimates for small and large time t so that the exponent n could be different for $t \to 0$ and for $t \to \infty$. Another method of doing so will be considered in Sections 6.3 and 6.2.

In 1987-89, Davies [41], [42], [43] proved that the on-diagonal upper bound (6.2) is equivalent to the log-*Sobolev inequality*: for any $f \in C_0^\infty(M)$, $f \geq 0$, and for any $\varepsilon > 0$,

$$\int f^2 \log \frac{f}{\|f\|_2} d\mu \leq \varepsilon \int |\nabla f|^2 \, d\mu + \beta(\varepsilon) \int f^2 d\mu \tag{6.10}$$

where $\|f\|_2 = \left(\int f^2 d\mu\right)^{1/2}$ and $\beta(\varepsilon) = C - \frac{n}{4}\log\varepsilon$. Davies also created a powerful method of proving the off-diagonal upper bounds like (6.9) using (6.10), which is called the semigroup perturbation method. A detailed account of it can be found in [43]. In the present paper, we have focused on two more recent methods of obtaining the Gaussian bounds - one based on the Davies inequality (3.5) and on the mean value property (5.17), and the other based on Ushakov's argument, which was stated in Corollary 5.5.

In 1994, Carron [20] and the author [69] proved that the on-diagonal upper bound (6.2) is equivalent to the *Faber-Krahn inequality:* for all precompact open sets $\Omega \subset M$,

$$\lambda_1(\Omega) \geq c\mu(\Omega)^{-2/n}, \tag{6.11}$$

where $\lambda_1(\Omega)$ is the lowest eigenvalue of the Dirichlet Laplace operator in Ω. The classical theorem of Faber and Krahn says that (6.11) holds in $\mathbb{R}^n$ with the constant c such that the equality in (6.11) is attained when Ω is a ball. In general, we do not need a sharp constant in (6.11) to obtain the heat kernel estimates.

By the variational principle, we have

$$\lambda_1(\Omega) = \inf_{\substack{f \in C_0^\infty(\Omega) \\ f \not\equiv 0}} \frac{\int_\Omega |\nabla f|^2 \, d\mu}{\int_\Omega f^2 d\mu}. \tag{6.12}$$

Hence, (6.11) can be rewritten as

$$\int_\Omega |\nabla f|^2 \, d\mu \geq c\mu(\Omega)^{-2/n} \int_\Omega f^2 d\mu, \quad \forall f \in C_0^\infty(\Omega). \tag{6.13}$$

It is not difficult to deduce the Nash inequality (6.8) directly from (6.13) - see Lemma 6.3 below.

Hence, we have the following equivalences:

$$\begin{array}{ccc}
\boxed{\text{log-Sobolev inequality (6.10)}} & \Leftrightarrow & \boxed{\text{Sobolev inequality (6.3)}} \\
\Updownarrow & & \Updownarrow \\
\boxed{\text{Off-diagonal Gaussian bound (6.9)}} & \Leftrightarrow & \boxed{\text{On-diagonal bound (6.2)}} \\
\Updownarrow & & \Updownarrow \\
\boxed{\text{Faber-Krahn inequality (6.11)}} & \Leftrightarrow & \boxed{\text{Nash inequality (6.8)}}
\end{array}$$

In the next sections, we will discuss similar relationships between more general heat kernel upper bounds and modifications of the Faber-Krahn inequality.

6.2 Arbitrary decay of the heat kernel

It is natural to ask what geometric or functional-analytic properties of the manifold M are responsible for the heat kernel bound as follows:

$$p(t,x,x) \leq \frac{C}{f(t)}, \quad \forall x \in M, \ t > 0, \tag{6.14}$$

where $f(t)$ is a prescribed[2] increasing function on $(0, \infty)$. The case $f(t) = t^{n/2}$ was considered above. However, there are plenty of simple examples of manifolds where such a function is not enough to describe the heat kernel behaviour. To start with, let us consider the manifolds $M = \mathbb{R}^m \times \mathbb{S}^k$ of the dimension $n = m + k$. Since the local structure of M is similar to that of $\mathbb{R}^n$, one may expect that, for short time t, we have $p(t,x,x) \asymp t^{-n/2}$ like in $\mathbb{R}^n$ (cf. (5.24)). However, in the large scale, M resembles $\mathbb{R}^m$ and, by (2.24), the long time asymptotic of $p(t,x,x)$ also looks like in $\mathbb{R}^m$. This motivates considering the following function

$$f(t) = \begin{cases} t^{n/2}, & t \leq 1, \\ t^{m/2}, & t > 1. \end{cases} \tag{6.15}$$

[2] As Proposition 5.14 says, $p(t,x,x)$ decays at most exponentially as $t \to \infty$. Therefore, $f(t)$ should grow at most exponentially, too.

On the hyperbolic space, the heat kernel decays exponentially in time as is seen from (1.2). One may presume that there are manifolds with superpolynomial but subexponential decay of $p(t,x,x)$ as $t\to\infty$, and this is true. This motivates us to consider the function

$$f(t)=\begin{cases} t^{n/2}, & t\leq 1,\\ \exp\left(t^{\alpha}\right), & t>1.\end{cases} \tag{6.16}$$

It is natural to try and extend the results of the preceding section to a wider class of functions f . The extension of the log-Sobolev inequality matching rather general $f(t)$ was obtained by Davies and can be found in his book [43]. A generalized Faber-Krahn inequality equivalent in some sense to (6.14), was obtained by the author [69] and will be discussed below. Finally, a generalized Nash inequality, also equivalent to (6.14), is due to Coulhon [35]. It seems that a proper generalization of the Sobolev inequality is not know yet (see [21], though).

Suppose that M is connected, non-compact and geodesically complete, and let Ω be a precompact region in M with smooth boundary. By (2.13), the long time asymptotic of $p_\Omega(t,x,x)$ reads as follows:

$$p_\Omega(t,x,x)\sim\exp\left(-\lambda_1\left(\Omega\right)t\right)\phi_1^2(x),\quad t\to\infty. \tag{6.17}$$

One may want to pass to the limit in (6.17) as $\Omega\to M$. Since $\lambda_1\left(\Omega\right)$ is decreasing on enlargement of Ω, the limit $\lim_{\Omega\to M}\lambda_1\left(\Omega\right)$ exists and coincides with the spectral radius $\lambda_1\left(M\right)$ (see (3.10)). If $\lambda_1\left(M\right)>0$ then one may expect that $p(t,x,x)$ behaves like $\exp\left(-\lambda_1(M)t\right)$ as $t\to\infty$. Indeed, (5.7) and (5.4) imply

$$p(t,x,x)\leq\exp\left(-\lambda_1\left(M\right)(t-t_0)\right)p(t_0,x,x). \tag{6.18}$$

This estimate is good when $\lambda_1\left(M\right)>0$ (cf. (5.43)) but becomes trivial if $\lambda_1(M)=0$. As the matter of fact, $\lambda_1(M)=0$ for all geodesically complete manifolds with subexponential volume growth (which follows from the theorem of Brooks [17]). The latter means that, for some $x\in M$,

$$V(x,r)=\exp\left(o(r)\right),\quad r\to\infty.$$

Hence, the case $\lambda_1(M)=0$ is most interesting from our point of view. One may wonder, if the rate of convergence of $\lambda_1(\Omega)$ to 0 as $\Omega\to M$ affects the rate of convergence of $p(t,x,x)$ to 0 as $t\to\infty$. In fact, it does if one understands the former as *a Faber-Krahn type inequality*

$$\lambda_1\left(\Omega\right)\geq\Lambda(\mu(\Omega)), \tag{6.19}$$

where Λ is a positive decreasing function on $(0,\infty)$. As we have mentioned in the previous section, (6.19) is true on $\mathbb{R}^n$ with the function $\Lambda(v)=cv^{-2/n}$. It turns out that inequality (6.19) can be proved in many interesting cases with various functions Λ. We will call Λ a *Faber-Krahn function* of M, assuming that (6.19) holds for all precompact $\Omega\subset M$.

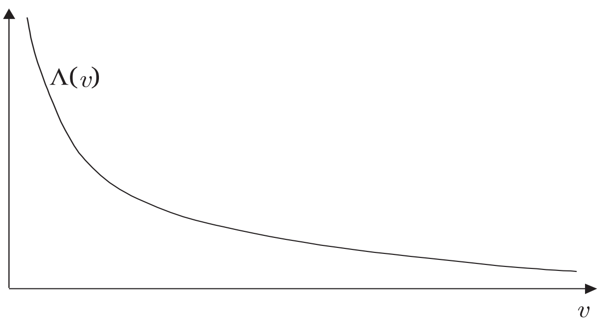

Figure 10 Example of a Faber-Krahn function

Theorem 6.2 *([69]) Assume that manifold M admits a Faber-Krahn function Λ. Let us define the function $f(t)$ by*

$$t=\int_0^{f(t)}\frac{dv}{v\Lambda(v)}, \tag{6.20}$$

assuming the convergence of the integral in (6.20) at 0*. Then, for all* $t>0$*,* $x\in M$*, and* $\varepsilon>0$*,*

$$p(t,x,x)\leq\frac{2\varepsilon^{-1}}{f((1-\varepsilon)\,t)}. \tag{6.21}$$

Examples: 1. If $\Lambda(v)=cv^{-2/n}$ then (6.20) yields $f(t)=c't^{n/2}$. Hence, (6.21) amounts to (6.2).

2. Let

$$\Lambda(v)\asymp\begin{cases}v^{-2/n}, & v\leq 1,\\ v^{-2/m}, & v>1.\end{cases} \tag{6.22}$$

For example, the manifold $M=K\times\mathbb{R}^m$, where K is a compact manifold of the dimension $n-m$, admits the Faber-Krahn function (6.22) (see Section 7.5). Then (6.20) gives

$$f(t)\asymp\begin{cases}t^{n/2}, & t\leq 1,\\ t^{m/2}, & t>1,\end{cases}$$

and

$$\sup_x p(t,x,x)\leq\frac{c}{t^{m/2}},\quad\forall t>1.$$

3. Assume

$$\Lambda(v)\asymp\log^{-\alpha}v,\quad v>2,$$

and $\Lambda(v)\asymp v^{-2/n}$ for $v<2$ (see Section 7.6 for examples of manifolds with this Λ). Then, for large t,

$$f(t)\asymp c_1\exp\left(c_2t^{\frac{1}{1+\alpha}}\right)$$

and

$$\sup_x p(t,x,x)\leq C\exp\left(-ct^{\frac{1}{1+\alpha}}\right).$$

4. Let us take

$$\Lambda(v)\equiv\lambda_1(M),\quad v>1,$$

and $\Lambda(v)\asymp v^{-2/n}$ for $v<1$ (note that the constant function $\Lambda(v)\equiv\lambda_1(M)$ satisfies (6.19) but the integral (6.20) diverges, so we have to modify it near $v=0$). Then, for large t,

$$f(t)\asymp\exp\left(\lambda_1(M)t\right)$$

and

$$\sup_x p(t,x,x)\leq C\exp\left(-\left(\lambda_1(M)-\varepsilon\right)t\right).$$

In fact, in this case ε can be taken 0 (this can be seen from the proof below or from (6.18)).

Proof of Theorem 6.2. Fix a point $y\in M$. We will prove that, for any precompact open set Ω with smooth boundary,

$$p_\Omega(t,y,y)\leq\frac{C_\varepsilon}{f((1-\varepsilon)\,t)},$$

provided $y\in\Omega$. Let us start as in the proof of Theorem 6.1: denote $u(t,x)=p_\Omega(t,x,y)$,

$$J(t):=\int_\Omega u^2(t,x)d\mu(x)$$

and obtain

$$J'(t)=-2\int_\Omega|\nabla u|^2\,d\mu. \tag{6.23}$$

Next, we have to estimate $\int|\nabla u|^2\,d\mu$ from below via $\int u^2d\mu$. The simplest way to do so is by using the variational property of the first eigenvalue which gives

$$\int_\Omega|\nabla u|^2\,d\mu\geq\lambda_1\left(\Omega\right)\int_\Omega u^2d\mu\geq\Lambda(\mu(\Omega))\int_\Omega u^2d\mu.$$

However, this is not suitable for us because the resulting estimate of u will depend on Ω. The following lemma provides a more sophisticated way of applying (6.19).

Lemma 6.3 *Assuming that (6.19) holds, we have, for any non-negative function* $u \in C^2(\Omega) \cap C(\overline{\Omega})$ *vanishing on* $\partial\Omega$,

$$\int |\nabla u|^2 \geq (1-\varepsilon)\left(\int u^2\right)\Lambda\left(\frac{2}{\varepsilon}\frac{\left(\int u\right)^2}{\int u^2}\right), \tag{6.24}$$

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

Remark 6.4 If $\Lambda(v) = cv^{-2/n}$ then (6.24) becomes the Nash inequality (6.8). Hence, (6.24) can be considered as a generalized Nash inequality.

Proof. The proof follows the argument of Gushchin [80]. Denote for simplicity $A = \int u d\mu$ and $B = \int u^2 d\mu$. For any positive s, we have the obvious inequality

$$u^2 \leq (u-s)_+^2 + 2su,$$

which implies, by integration,

$$B \leq \int_{\{u>s\}} (u-s)^2 d\mu + 2sA. \tag{6.25}$$

Applying the Faber-Krahn inequality (6.19) in the region $\Omega_s := \{u > s\}$ (observe that $u - s$ vanishes on the boundary $\partial\Omega_s$), we get

$$\int_{\Omega_s} (u-s)^2 d\mu \leq \frac{\int_{\Omega_s} |\nabla u|^2 d\mu}{\Lambda(\mu(\Omega_s))}. \tag{6.26}$$

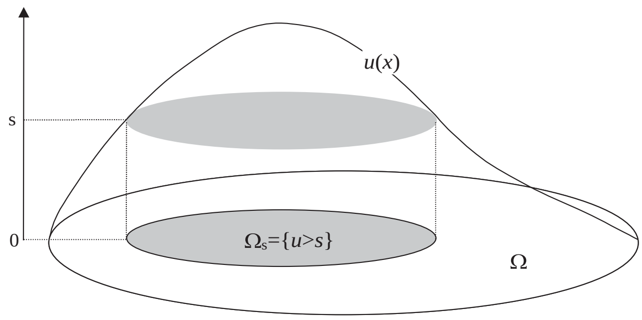

Figure 11 Applying a Faber-Krahn inequality for the region Ω_s

Unlike Ω, the region Ω_s admits estimating of its volume via the function u, as follows

$$\mu(\Omega_s) \leq \frac{1}{s}\int_\Omega u\, d\mu = s^{-1}A.$$

Hence, (6.25) and (6.26) imply

$$B \leq \frac{\int_{\Omega_s} |\nabla u|^2 d\mu}{\Lambda(s^{-1}A)} + 2sA$$

whence

$$\int_\Omega |\nabla u|^2 d\mu \geq (B - 2sA)\Lambda\left(s^{-1}A\right).$$

Taking here $s = \frac{\varepsilon B}{2A}$, we finish the proof. ■

Applying Lemma 6.3 to estimate the right hand side of (6.23) and taking into account that

$$\int u(t,x)d\mu(x) \leq 1,$$

we obtain

$$J' \leq -2\,(1-\varepsilon)\,J\Lambda\left(\frac{2}{\varepsilon}\frac{1}{J}\right).$$

Dividing this inequality by the right hand side, integrating it against dt from 0 to t and changing the variables $v = 2\varepsilon^{-1}J^{-1}$, we obtain

$$\int_0^{2\varepsilon^{-1}J^{-1}} \frac{dv}{v\Lambda(v)} \geq 2\,(1-\varepsilon)\,t$$

whence, by the definition (6.20) of function f,

$$J(t) \leq \frac{2\varepsilon^{-1}}{f(2(1-\varepsilon)t)}.$$

We are left to notice that $J(t) = p_\Omega\,(2t, y, y)$, and (6.21) follows. ■

If the function Λ satisfying the hypotheses of Theorem 6.2 is continuous then $f(t) \in C^1(\mathbb{R}_+)$ and

$$f' > 0, \quad f(0) = 0, \quad f(\infty) = \infty \quad \text{and} \quad \frac{f'}{f} \text{ is non-increasing.} \tag{6.27}$$

Conversely, if $f \in C^1\,(\mathbb{R}_+)$ satisfies (6.27) then Λ from (6.20) can be recovered by

$$\Lambda(f(t)) = \frac{f'}{f}. \tag{6.28}$$

The following Theorem is almost converse to Theorem 6.2.

Theorem 6.5 *([69]) Let the heat kernel on the manifold M admit the following estimate*

$$\sup_x p(t,x,x) \leq \frac{1}{f(t)}, \quad \forall t > 0, \tag{6.29}$$

where $f \in C^1\,(\mathbb{R}_+)$ satisfies (6.27) and certain regularity condition below. Then M admits the Faber-Krahn function $c\Lambda(v)$ where Λ is defined by (6.28).

Moreover, for any precompact region $\Omega \subset M$ and any integer $k \geq 1$,

$$\lambda_k(\Omega) \geq c\Lambda\left(\frac{\mu\,(\Omega)}{k}\right). \tag{6.30}$$

We say that a function $g(t)$ has *at most polynomial decay* if, for some $\alpha > 0$ and $a \in [1,2]$,

$$g(at) \geq \alpha g(t), \quad \forall t > 0. \tag{6.31}$$

The the regularity condition in the statement of Theorem 6.5 is as follows: the function $g := (\log f)'$ has at most polynomial decay. For example, the latter holds if, for some large $A > 0$,

$$\frac{f''}{f'} \geq \frac{f'}{f} - \frac{A}{t}.$$

All examples of f considered above, satisfy this condition. On the contrary, $f(t) = 1 - e^{-t}$ does not satisfy it.

Proof. The hypotheses (6.29) implies $p_\Omega(t,x,x) \leq \frac{1}{f(t)}$ whence

$$\int_\Omega p_\Omega(t,x,x)d\mu(x) \leq \frac{\mu(\Omega)}{f(t)}.$$

On the other hand, by the eigenfunction expansion (2.9),

$$\int_\Omega p_\Omega(t,x,x)d\mu(x) = \int_\Omega \sum_{i=1}^\infty e^{-\lambda_i(\Omega)t}\phi_i^2(x)d\mu(x) = \sum_{i=1}^\infty e^{-\lambda_i(\Omega)t}.$$

The right hand side here is bounded from below by $ke^{-\lambda_k(\Omega)t}$, whence

$$\frac{\mu(\Omega)}{f(t)} \geq ke^{-\lambda_k(\Omega)t}$$

and

$$\lambda_k(\Omega) \geq \frac{1}{t} \log \frac{kf(t)}{\mu(\Omega)}. \tag{6.32}$$

This inequality holds for all $t > 0$ so that we can choose t. Let us find t from the equation

$$f(t/2) = \mu(\Omega)/k.$$

For this t, we obtain from (6.32)

$$\lambda_k(\Omega) \geq \frac{1}{t} \left(\log f(t) - \log f(t/2)\right) = \frac{1}{2} g(\theta),$$

where $g := (\log f)'$ and $\theta \in (t/2, t)$. By the regularity condition (6.31), we have $g(\theta) \geq \alpha g(t/2)$. Finally, we apply (6.28):

$$g(t/2) = \frac{f'(t/2)}{f(t/2)} = \Lambda\left(f(t/2)\right) = \Lambda(\frac{\mu(\Omega)}{k})$$

whence

$$\lambda_k(\Omega) \geq \frac{\alpha}{2} \Lambda(\frac{\mu(\Omega)}{k}),$$

which was to be proved. ■

It is follows from Theorems 6.2 and 6.5 that the heat kernel upper bound (6.29) is equivalent to the certain Faber-Krahn type inequality, up to some constant multiples. Clearly, the generalized Nash inequality (6.24) involved in the proof of Theorem 6.2, is also equivalent to each of these hypotheses. The latter was further developed in an abstract semigroup setting by Coulhon [35]. He also gave another proof of the first part of Theorem 6.5 avoiding usage of the eigenfunction expansion.

Putting together Theorems 6.2 and 6.5, we obtain

Corollary 6.6 *Suppose that the function Λ satisfies the hypotheses of Theorems 6.2 and 6.5. If, for any precompact open set $\Omega \subset M$,*

$$\lambda_1(\Omega) \geq \Lambda(\mu(\Omega)) \tag{6.33}$$

then, for all integers $k \geq 1$,

$$\lambda_k(\Omega) \geq c\Lambda(C\mu(\Omega)). \tag{6.34}$$

For example, for the Euclidean function $\Lambda(v) = cv^{-2/n}$, we obtain

$$\lambda_k(\Omega) \geq c' \left(\frac{k}{\mu(\Omega)}\right)^{2/n}.$$

Note that (6.34) does not follow from (6.33) for an *individual* set Ω: it is essential that (6.33) holds for *all* Ω.

By reverting the Faber-Krahn inequality (6.33), it is possible to prove some lower bounds of the heat kernel - see [36, Theorem 3.2].

6.3 Localized upper estimate

We consider here the localized version of Theorem 6.1.

Theorem 6.7 *([66], [69]) Suppose that, for some $x \in M$ and $r > 0$, the following Faber-Krahn inequality holds: for any precompact open set $\Omega \subset B(x,r)$*

$$\lambda_1(\Omega) \geq a\mu(\Omega)^{-2/n}, \tag{6.35}$$

where $a > 0$ and $n > 0$. Then, for any $t > 0$,

$$p(t,x,x) \leq \frac{Ca^{-n/2}}{\min(t,r^2)^{n/2}}, \tag{6.36}$$

where $C = C(n)$.

Remark 6.8 This theorem contains Theorem 6.1 as $r \to \infty$, taking into account that (6.35) is equivalent to (6.3). However, the method of proof of Theorems 6.1 and 6.2 does not work in the setting of Theorem 6.7 because it requires (6.35) for all Ω, not only for those in $B(x,r)$.

The coefficient a in (6.36) can be absorbed into the constant C. However, by varying the ball $B(x,r)$, we may have different a for different balls so that the exact dependence on a in (6.36) may be crucial. In the next section we will consider a setting where a depends explicitly on $B(x,r)$.

Proof. We start with the following mean-value type inequality.

Lemma 6.9 *Suppose that the Faber-Krahn inequality (6.35) holds for any precompact open set $\Omega \subset B(x,r)$. Then, for any $\tau \in (0,r^2]$, $t \geq \tau$ and for any positive solution u of the heat equation in the cylinder $(t-\tau,t] \times B(x,\sqrt{\tau})$, we have*

$$u(t,x) \leq \frac{Ca^{-n/2}}{\tau^{1+n/2}} \int_{t-\tau}^{t} \int_{B(x,\sqrt{\tau})} u(s,y)d\mu(y)ds, \tag{6.37}$$

where $C = C(n)$.

Remark 6.10 The term $\tau^{1+n/2}$ is proportional to the volume of the cylinder of the height τ and of the base being a ball of radius $\sqrt{\tau}$ in $\mathbb{R}^n$. This reflects the fact that the Faber-Krahn inequality (6.35) is optimal in $\mathbb{R}^n$ but may not be optimal in M. A different type of the mean-value property (5.17) related to the volume $V(x,\sqrt{\tau})$ on M was considered in Section 5.2 (see also the next section).

The proof of (6.37) consists of two steps. The first step is the L^2-mean-value inequality, that is, (6.37) for u^2 instead of u, which was proved in [67, Theorem 3.1]. Alternatively, the L^2-mean-value inequality follows from the first part of the Moser iteration argument [106], given the equivalence of (6.35) and certain Sobolev inequality (see [20]). The second step is to derive (6.37) from the L^2-mean-value inequality. This is done by using the argument of Li and Schoen [95] (see also [97] and [37]).

The estimate (6.36) follows from Lemma 6.9 similarly to the first part of the proof of Theorem 5.8. Indeed, integrating in time the inequality

$$\int_M p(s,x,y)d\mu(y) \leq 1$$

we obtain, for all $t \geq \tau > 0$,

$$\int_{t-\tau}^{t} \int_M p(s,x,y)d\mu(y) \leq \tau.$$

Hence (6.37) yields, for $u = p(\cdot, x, \cdot)$ and for $\tau \in (0, r^2]$,

$$p(t,x,x) \leq \frac{Ca^{-n/2}}{\tau^{1+n/2}} \int_{t-\tau}^{t} \int_M p(s,x,y)d\mu(y) \leq \frac{Ca^{-n/2}}{\tau^{n/2}}.$$

Clearly, (6.36) follows if we choose $\tau = \min(t, r^2)$. ■

Corollary 6.11 *Suppose that, for all $x \in M$ and some $r > 0$, the Faber-Krahn inequality (6.35) holds, for any precompact open set $\Omega \subset B(x,r)$. Then, for any $D > 2$ and all $x, y \in M$, $t > 0$,*

$$p(t,x,y) \leq \frac{Ca^{-n/2}}{\min(t,r^2)^{n/2}} \exp\left(-\frac{d^2(x,y)}{2Dt}\right), \tag{6.38}$$

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

The estimate (6.38) follows from (6.36) and from the inequality (5.14) of Corollary 5.5. If we use (5.15) instead of (5.14) then we obtain

$$p(t,x,y) \leq \frac{Ca^{-n/2}e^{\lambda_1(M)t_0}}{\min(t,t_0)^{n/2}} \exp\left(-\lambda_1(M)t - \frac{d^2(x,y)}{2Dt}\right) \tag{6.39}$$

where $t_0 = r^2$. By absorbing a and t_0 into C, we can rewrite (6.39) as follows:

$$p(t,x,y) \leq \frac{C'}{\min(t,1)^{n/2}} \exp\left(-\lambda_1(M)t - \frac{d^2(x,y)}{2Dt}\right). \tag{6.40}$$

6.4 Relative Faber-Krahn inequality and the decay of the heat kernel as $V(x, \sqrt{t})^{-1}$.

We return here to heat kernel upper bound

$$p(t,x,x) \leq \frac{C}{V(x,\sqrt{t})}, \tag{6.41}$$

which was discussed already in Section 5.17. Similarly to the equivalence

On-diagonal bound (6.2)$\Longleftrightarrow$Faber-Krahn inequality (6.11)

mentioned in Section 6.1, we will show that (6.41) is “almost” equivalent to *the relative Faber-Krahn inequality* defined as follows.

Definition 6.12 *We say that M admits* the relative Faber-Krahn inequality *if, for any ball $B(x,r) \subset M$ and for any precompact open set $\Omega \subset B(x,r)$,*

$$\lambda_1(\Omega) \geq \frac{b}{r^2}\left(\frac{V(x,r)}{\mu(\Omega)}\right)^{\nu}, \tag{6.42}$$

with some positive constants b, ν.

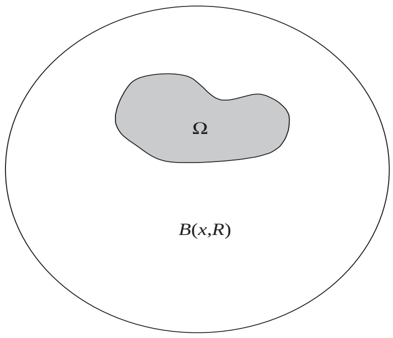

Figure 12 Subset Ω of the ball $B(x,R)$

It is easy to see that (6.42) holds in $\mathbb{R}^n$ with $\nu = 2/n$. It is possible to prove that the relative Faber-Krahn inequality holds on any geodesically complete manifold of non-negative Ricci curvature - see [67]. In general, a non-negatively curved manifold admits no *uniform* Faber-Krahn function in the spirit of Section 6.2. The inequality (6.42) was designed to overcome this difficulty. It provides a lower bound for $\lambda_1(\Omega)$, which takes into account not only volume $\mu(\Omega)$ but also *location* of the set Ω, via the ball $B(x,r)$.

We say that the volume function $V(x,r)$ satisfies *the doubling property* if, for some constant C,

$$V(x,2r) \le CV(x,r), \quad \forall x \in M, \ r > 0. \tag{6.43}$$

Now we can state the main theorem of this section.

Theorem 6.13 *([69, Proposition 5.2]) Let M be a geodesically complete manifold.*

If M admits the relative Faber-Krahn inequality then the heat kernel satisfies the upper bound (6.41), for all $x \in M$ and $t > 0$, and the volume function $V(x,r)$ satisfies the doubling property (6.43).

Conversely, the heat kernel upper bound (6.41) and the doubling volume property (6.43) imply (6.42).

Proof. The implication (6.42)$\Longrightarrow$(6.41) follows from Theorem 6.7. Indeed, given a ball $B(x,r)$, we have, by (6.35), for any precompact open set $\Omega \subset B(x,r)$,

$$\lambda_1(\Omega) \ge a\mu(\Omega)^{-2/n}, \tag{6.44}$$

where $n = 2/\nu$ and

$$a = \frac{b}{r^2} V(x,r)^{2/n}. \tag{6.45}$$

Hence, Theorem 6.7 implies, for any $r > 0$,

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

Taking $r = \sqrt{t}$ and substituting a from (6.45) we obtain (6.41).

Another proof of (6.42)$\Longrightarrow$(6.41) follows by Theorem 5.8. Indeed, given (6.44), Lemma 6.9 implies that, for any positive solution u of the heat equation in the cylinder $(t-r^2,t] \times B(x,r)$ (assuming $\tau := r^2 \le t$),

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

Substituting a from (6.45), we obtain the mean-value property (MV) (see Definition 5.7). Hence, Theorem 5.8 can be applied and yields (6.41).

The implication (6.42)$\Longrightarrow$(6.43) is proved by the argument of Carron [20] - see [69, p.442]. The second part of Theorem 6.13 – the implication (6.41)+(6.43)$\Longrightarrow$(6.42), is proved similarly to Theorem 6.5 - see [69, p.443]. ■

The above proof together with Theorems 5.8 and 5.12 gives the following

Corollary 6.14 *The following implications hold*

$$\boxed{\textit{Relative Faber-Krahn inequality (6.42)}}$$
$$\Updownarrow$$
$$\boxed{\textit{Mean-value property } \text{(MV)} \textit{ and volume doubling (6.43).}}$$
$$\Updownarrow$$
$$\boxed{\textit{Gaussian upper bound (5.19) and volume doubling (6.43)}}$$
$$\Updownarrow$$
$$\boxed{\textit{On-diagonal upper bound (6.41) and volume doubling (6.43)}}$$
$$\Downarrow$$
$$\boxed{\textit{On-diagonal lower bound (5.40)}}$$

Another (direct) proof of the second equivalence was obtained by Li and Wang [97].

7 Isoperimetric inequalities

7.1 Isoperimetric inequalities and $\lambda_1(\Omega)$

Isoperimetric inequality relates the boundary area of regions to their volume. We say that manifold M admits *the isoperimetric function* I if, for any precompact open set $\Omega \subset M$ with smooth boundary,

$$\sigma(\partial\Omega) \geq I(|\Omega|), \tag{7.1}$$

where

$$|\Omega| := \mu(\Omega).$$

For example, $\mathbb{R}^n$ admits the isoperimetric function $I(v) = c_n v^{\frac{n-1}{n}}$. Indeed, let $\Omega^* \subset \mathbb{R}^n$ be a ball of the same volume as Ω and let r be its radius. Then, by the classical isoperimetric inequality,

$$\sigma(\partial\Omega) \geq \sigma(\partial\Omega^*) = \omega_n r^{n-1} = c_n \left(\frac{\omega_n}{n} r^n\right)^{\frac{n-1}{n}} = c\,|\Omega^*|^{\frac{n-1}{n}} = c_n\,|\Omega|^{\frac{n-1}{n}}.$$

Other examples of isoperimetric functions will be shown below.

It turns out that the isoperimetric inequality (7.1) implies a Faber-Krahn inequality (6.19). The next statement is a version of Cheeger's inequality [26].

Proposition 7.1 *Let $I(v)$ be a non-negative continuous function on $\mathbb{R}_+$ such that $I(v)/v$ is non-increasing. Assume that M admits the isoperimetric function I. Then M admits the Faber-Krahn function*

$$\Lambda(v) := \frac{1}{4}\left(\frac{I(v)}{v}\right)^2. \tag{7.2}$$

For example, if $I(v) = cv^{\frac{n-1}{n}}$ then (7.2) yields $\Lambda(v) = \frac{c^2}{4} v^{-2/n}$.

Proof. Given a non-negative function $f \in C_0^\infty(\Omega)$, we denote

$$\Omega_s = \{x : f(x) > s\}.$$

By Sard's theorem, the boundary $\partial\Omega_s$ is smooth, for almost all s, so that we can apply the isoperimetric inequality (7.1) for Ω_s and obtain

$$\sigma(\partial\Omega_s) \geq I(|\Omega_s|) \tag{7.3}$$

for almost all s. Next, we use the co-area formula

$$\int_M |\nabla f|\, d\mu = \int_0^\infty \sigma(\partial\Omega_s)\, ds, \tag{7.4}$$

which implies with (7.3) and the non-increasing of $I(v)/v$,

$$\begin{aligned} \int_M |\nabla f|\, d\mu &\geq \int_0^\infty I(|\Omega_s|) ds \\ &= \int_0^\infty \frac{I(|\Omega_s|)}{|\Omega_s|} |\Omega_s|\, ds \\ &\geq \frac{I(|\Omega|)}{|\Omega|} \int_0^\infty |\Omega_s|\, ds \\ &= \frac{I(|\Omega|)}{|\Omega|} \int_M f\, d\mu. \end{aligned} \tag{7.5}$$

By the Cauchy-Schwarz inequality, we have

$$\int_M \left|\nabla f^2\right| d\mu = 2\int_M f\,|\nabla f| \leq 2\left[\int_M f^{\,2}\,d\mu \int_M |\nabla f|^2\,d\mu\right]^{1/2}. \tag{7.6}$$

Applying (7.5) to f^2 instead of f and by (7.6), we obtain

$$\frac{I(|\Omega|)}{|\Omega|}\int_M f^{\,2}\,d\mu \leq \int_M \left|\nabla f^2\right| d\mu \leq 2\left[\int_M f^{\,2}\,d\mu \int_M |\nabla f|^2\,d\mu\right]^{1/2}$$

whence

$$\left(\frac{I(|\Omega|)}{|\Omega|}\right)^2 \int_M f^{\,2}\,d\mu \leq 4\int_M |\nabla f|^2\,d\mu$$

and

$$\lambda_1(\Omega) \geq \frac{1}{4}\left(\frac{I(|\Omega|)}{|\Omega|}\right)^2,$$

which was to be proved. ■

Combining Proposition 7.1 with Theorem 6.2 and Corollary 5.5, we obtain

Corollary 7.2 *Assume that manifold M admits a non-negative continuous isoperimetric function $I(v)$ such that $I(v)/v$ is non-increasing. Let us define the function $f(t)$ by*

$$t = 4\int_0^{f(t)} \frac{vdv}{I^2(v)}, \tag{7.7}$$

assuming the convergence of the integral in (7.7) at 0. Then, for all $x \in M$, $t > 0$ and $\varepsilon > 0$,

$$p(t,x,x) \leq \frac{2\varepsilon^{-1}}{f((1-\varepsilon)\,t)}. \tag{7.8}$$

Furthermore, if the function f satisfies in addition the regularity condition (5.11) then, for all $x, y \in M$, $t > 0$, $D > 2$ and some $\varepsilon > 0$,

$$p(t,x,y) \leq \frac{C}{f(\varepsilon t)}\exp\left(-\frac{d^2(x,y)}{2Dt}\right). \tag{7.9}$$

In the next sections, we will show examples of manifolds satisfying certain isoperimetric and Faber-Krahn inequalities where the heat kernel estimates given by Theorems 6.2, 6.7, 6.13 and Corollaries 6.11, 7.2 can be applied.

7.2 Isoperimetric inequalities and the distance function

Here we mention a certain method of proving isoperimetric inequalities, which was introduced by Michael and Simon [104]. Suppose that we have a distance function $r(x,\xi)$ on M. This may be the Riemannian distance or a general distance function satisfying the usual axioms of the metric space, in particular, the triangle inequality. We will denote $r(x,\xi)$ by $r_\xi(x)$ to emphasize that it will be regarded as a function of x with a fixed (but arbitrary) ξ. It turns out that an isoperimetric inequality on M can be proved if one knows certain bounds for $|\nabla r_\xi|$ and Δr_ξ.

Theorem 7.3 *(Michael–Simon [104], Chung–Grigor'yan–Yau [33]) Let M be a geodesically complete Riemannian manifold of dimension $n > 1$. Suppose that $r_\xi(x)$ is a distance function on M such that, for all $\xi, x \in M$,*

$$|\nabla r_\xi(x)| \leq 1 \tag{7.10}$$

and

$$\Delta r_\xi^2(x) \geq 2n \tag{7.11}$$

(assuming that $r_\xi^2 \in C^2(M)$). Then M admits the isoperimetric function $I(v) = cv^{\frac{n-1}{n}}$ where $c = c_n > 0$.

Let us explain why (7.10) and (7.11) should be related to isoperimetric inequalities. Indeed, integrating (7.10) over a precompact region $\Omega \subset M$ with smooth boundary and using the Green formula (2.4), we obtain

$$2n\,|\Omega| = \int_\Omega \Delta(r_\xi^2)d\mu = 2\int_{\partial\Omega} r_\xi \frac{\partial r_\xi}{\partial \nu} d\sigma\,, \tag{7.12}$$

where ν is the outward normal vector field on $\partial\Omega$. With the obvious inequality $\frac{\partial r_\xi}{\partial \nu} \leq |\nabla r_\xi| \leq 1$, (7.12) implies

$$n\,|\Omega| \leq \left(\sup_\Omega r_\xi\right)\sigma(\partial\Omega). \tag{7.13}$$

This is already a weak form of isoperimetric inequality. A certain argument allows to extend (7.13) as to show the isoperimetric inequality

$$\sigma\left(\partial\Omega\right) \geq c\,|\Omega|^{\frac{n-1}{n}}\,.$$

See [104] or [33] for further details.

7.3 Minimal submanifolds

Let M be an n-dimensional submanifold of $\mathbb{R}^N$ with the Riemannian metric inherited from $\mathbb{R}^N$. Submanifold M is called *minimal* if its normal mean curvature vector $H(x) = (H_1(x), H_2(x), ..., H_N(x))$ vanishes for all $x \in M$ (see [113]). It turns out that already the minimality of M implies certain isoperimetric property.

Theorem 7.4 *(Bombieri – de Giorgi – Miranda [16]) Any n-dimensional minimal submanifold M admits the isoperimetric function $I(v) = cv^{\frac{n-1}{n}}$, $c > 0$.*

Proof. Consider the coordinate functions X_i in $\mathbb{R}^N$ as functions on M. Then $\Delta X_i = H_i(x)$ where Δ is the Laplacian on M (see [113, Theorem 2.4]). Let us denote by $r_\xi(x)$ the (extrinsic) Euclidean distance in $\mathbb{R}^N$ between the points $x, \xi \in M$. Shifting the coordinates $X_1, X_2, ..., X_N$ in $\mathbb{R}^N$ to have the origin ξ, we have

$$\Delta r_\xi^2 = \sum_{i=1}^N \Delta(X_i^2) = 2\sum_{i=1}^N X_i H_i + 2\sum_{i=1}^N |\nabla X_i|^2\,.$$

The term $\sum X_i H_i$ identically vanishes if M is minimal. The sum $\sum_{i=1}^N |\nabla X_i|^2$ is equal to n for *any* n-dimensional submanifold, which can be verified by a direct computation. Hence, we conclude

$$\Delta r_\xi^2 = 2n. \tag{7.14}$$

On the other hand, it is obvious that $|\nabla r_\xi| \leq 1$ because the extrinsic distance is majorized by the intrinsic Riemannian distance on M. Hence, we can apply Theorem 7.3 and conclude the proof. ■

Theorem 7.4 and Corollary 7.2 imply the following uniform upper bound for the heat kernel on M

$$p(t, x, y) \leq \frac{C}{t^{n/2}} \exp\left(-\frac{d^2(x, y)}{2Dt}\right). \tag{7.15}$$

7.4 Cartan-Hadamard manifolds

A manifold M is called *a Cartan-Hadamard manifold* if M is geodesically complete simply connected non-compact Riemannian manifold with non-positive sectional curvature. For example, $\mathbb{R}^n$ and $\mathbb{H}^n$ are Cartan-Hadamard manifolds.

Theorem 7.5 *(Hoffman – Spruck [84]) Any Cartan-Hadamard manifold M of the dimension n admits the isoperimetric function $I(v) = cv^{\frac{n-1}{n}}$, $c > 0$.*

This theorem can also be derived from Theorem 7.3. Indeed, denote by $r_\xi(x)$ the geodesic distance between the point x and ξ on M. If $M = \mathbb{R}^n$ then $\Delta r_\xi^2 = 2n$. For general Cartan-Hadamard manifold, the comparison theorem for the Laplacian implies $\Delta r_\xi^2 \geq 2n$ (see [122]), whereas $|\nabla r_\xi| \leq 1$ holds on any manifold.

Hence, the heat kernel estimate (7.15) is valid on Cartan-Hadamard manifolds, too. On the other hand, by Proposition 7.1, Cartan-Hadamard manifolds satisfy the hypotheses of Corollary 6.11. Therefore, (6.40) holds, that is,

$$p(t,x,y) \leq \frac{C}{\min\left(1, t^{n/2}\right)} \exp\left(-\lambda_1(M)t - \frac{d^2(x,y)}{2Dt}\right), \tag{7.16}$$

which can be better than (7.15) if $\lambda_1(M) > 0$.

McKean's theorem [103] says that if the sectional curvature of the Cartan-Hadamard manifold is bounded from above by $-K^2$ then

$$\lambda_1(M) \geq \frac{(n-1)^2}{4} K^2. \tag{7.17}$$

Indeed, consider again the Riemannian distance function $r_\xi(x)$. As Yau [139] showed, on such manifolds

$$\Delta r_\xi \geq (n-1)K, \tag{7.18}$$

away from ξ. Given a precompact open set $\Omega \subset M$ with smooth boundary, we choose $\xi \notin \overline{\Omega}$ and integrate (7.18) over Ω. By the Green formula 2.4, we obtain

$$\int_{\partial\Omega} \frac{\partial r_\xi}{\partial \nu} d\sigma \geq (n-1)K\,|\Omega|\,.$$

Since $\frac{\partial r_\xi}{\partial \nu} \leq |\nabla r_\xi| \leq 1$, we arrive to the isoperimetric inequality

$$\sigma(\partial\Omega) \geq (n-1)K\,|\Omega|\,,$$

whence (7.17) follows by Proposition 7.1.

Hence, (7.16) implies, for all $x, y \in M$, $t > 0$ and $D > 2$,

$$p(t,x,y) \leq \frac{C}{\min(1, t^{n/2})} \exp\left(-\frac{(n-1)^2}{4}K^2 t - \frac{d^2(x,y)}{2Dt}\right). \tag{7.19}$$

Let us compare (7.19) with the sharp uniform estimate of the heat kernel on the hyperbolic space $\mathbb{H}_K^n$ of the constant negative curvature $-K^2$ obtained by Davies and Mandouvalos [50]:

$$p(t,x,y) \asymp \frac{(1+d+t)^{\frac{n-3}{2}}(1+d)}{t^{n/2}} \exp\left(-\frac{(n-1)^2}{4}K^2 t - \frac{d^2}{4t} - \frac{n-1}{2}Kd\right), \tag{7.20}$$

where $d = d(x,y)$ (see [43] and [77] for the exact formula for the heat kernel on hyperbolic spaces; the estimate (7.20) admits a far reaching generalization for symmetric spaces - see [3]).

If $t \to \infty$ then (7.20) yields

$$p(t,x,x) \asymp t^{-3/2} \exp\left(-\frac{(n-1)^2}{4}K^2 t\right),$$

which is better than (7.19) by the factor $t^{-3/2}$. The geometric nature of this factor is still unclear.

Another difference between (7.19) and (7.20) is the constant $D > 2$ in the Gaussian term. It is possible to put $D = 2$ in (7.19) at expense of the polynomial correction term, as in Theorem 5.9 – see [68, p.254] or [69, Theorem 5.2].

Yet another difference between (7.19) and (7.20) is the third term $\frac{n-1}{2}Kd$ in the exponential. It does not play a significant role for the heat kernel in the hyperbolic space because it is dominated by the sum of two other terms in the exponential (7.20). However, it is possible to introduce a similar term for general Cartan-Hadamard manifolds, and it may be leading if the curvature goes to $-\infty$ fast enough as $x \to \infty$.

Fix a point $o \in M$ and denote[3]

$$L(r) := \lambda_1(M \setminus \overline{B(o,r)}). \tag{7.21}$$

Clearly, $L(r)$ is increasing in r and $L(0) = \lambda_1(M)$. If the sectional curvature outside the ball $B(o,r)$ is bounded above by $-K^2(r)$ (where $K(r)$ is positive and increasing) then a modification of (7.17) says that

$$L(r) \geq \frac{(n-1)^2}{4} K(r)^2. \tag{7.22}$$

Theorem 7.6 *([69, Theorem 5.3]) Let M be a Cartan-Hadamard manifold of the dimension n and $o \in M$. Then, for all $t > 0$, $x \in M \setminus B(o, \sqrt{t})$, $c \in (0,1)$ and some $\varepsilon = \varepsilon(c) > 0$,*

$$p(t,o,x) \leq \frac{C}{t^{n/2}} \exp\left(-c\lambda_1(M)t - c\frac{d^2}{4t} - \varepsilon d\sqrt{L(cd)}\right), \tag{7.23}$$

where $d = \operatorname{dist}(o,x)$ and $C = C(c,n)$.

Proof of Theorem 7.6 is similar to that of Theorem 6.7 but uses a more general mean-value type inequality than Lemma 6.9 – see [69] for details. It is not clear whether one can put $c = 1$ here.

As a consequence we see that if the sectional curvature *outside* the ball $B(o,r)$ is bounded *above* by $-K^2(r)$ then (7.23) and (7.22) yield

$$p(t,o,x) \leq \frac{C}{t^{n/2}} \exp\left(-c\lambda_1(M)t - c\frac{d^2}{4t} - \varepsilon K(cd)d\right). \tag{7.24}$$

In particular, if $K(r) \gg r$ then the term $K(cd)d$ is leading as $d \to \infty$.

It is possible to prove the following matching lower bound. Assume that the sectional curvature *inside* the ball $B(o,r)$ is bounded *below* by $-K^2(r)$. Then we claim that, for all $t > 0$, $x \in M$ and $\varepsilon > 0$,

$$p(t,o,x) \geq \frac{c}{t^{n/2}} \exp\left(-\left(\lambda_1(M) + \varepsilon\right)t - C\frac{d^2}{4t} - CK(d+C)d\right), \tag{7.25}$$

where $c = c(o,\varepsilon) > 0$ (cf. (7.28) below).

Comparison of (7.24) and (7.25) shows that there is a big gap in the values of the constants in the upper and lower bounds. The problem of obtaining optimal heat kernel estimates when the curvature grows to $-\infty$ faster than quadratically in r, is not well understood.

Another interesting consequence of (7.23) is related to *the essential spectrum* of the operator Δ_M. Denote by $\lambda_{ess}(M)$ the bottom of the essential spectrum of $-\Delta_M$ in $L^2(M,\mu)$. It is known and is due to Donnelly [58] that, on any complete manifold,

$$\lambda_{ess}(M) = \lim_{r\to\infty} L(r), \tag{7.26}$$

where $L(r)$ is defined by (7.21). It is possible to derive from (7.23) and (7.26) that

$$\limsup_{d\to\infty} \frac{1}{d} \sup_{t>0} \log p(t,o,x) \leq -C\left(\sqrt{\lambda_1(M)} + \sqrt{\lambda_{ess}(M)}\right), \tag{7.27}$$

[3]The notation $\lambda_1(\Omega)$ (where Ω is not necessarily compact) is defined by (6.12). This is the bottom of the spectrum of the operator $-\Delta_\Omega$ in $L^2(\Omega,\mu)$.

where $d = d(x, o)$ (see [69, Corollary 5.1]) and $C > 0$ is an absolute constant. It would be interesting to understand to what extent this inequality is sharp, in particular, what is a sharp value of C. For the hyperbolic space, equality is attained in (7.27) with $C = 1$.

7.5 Manifolds of bounded geometry

We say that a manifold M has *bounded geometry* if its Ricci curvature is uniformly bounded below and if its injectivity radius is bounded away from 0. The hypothesis of bounded geometry implies that, for some $r_0 > 0$, all balls $B(x, r_0)$, $x \in M$, are uniformly quasi-isometric to the Euclidean ball $B_E(r_0) \subset \mathbb{R}^n$, where $n = \dim M$. The term "quasi-isometric" means that there is a diffeomorphism between $B(x, r_0)$ and $B_E(r_0)$ which changes the distances at most by a constant factor, and the word "uniform" refers to the fact that this constant factor is the same for all $x \in M$.

In other words, the manifold M looks like being patched from slightly distorted copies of the ball $B_E(r_0)$. Clearly, a manifold of bounded geometry is geodesically complete.

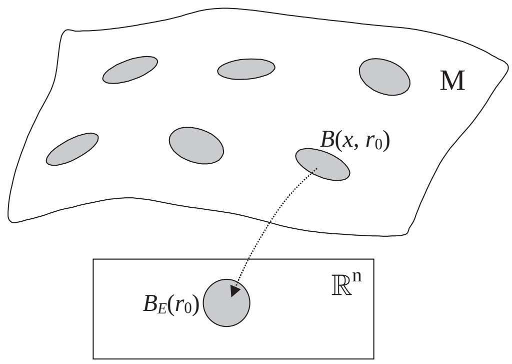

Figure 13 Manifold of bounded geometry is "patched" from slightly distorted Euclidean balls

The hypotheses of Corollary 6.11 are satisfied on the manifold M of bounded geometry. Hence, the upper bound (6.40) (the same as (7.16)) holds on M. Using Proposition 5.14 and the standard chain argument with the local Harnack inequality, it is possible to prove the following lower bound

$$p(t, x, y) \geq c_{x,\varepsilon} \exp\left(-(\lambda_1(M) + \varepsilon)t - C\frac{d^2(x, y)}{t}\right), \tag{7.28}$$

for any $\varepsilon > 0$ and all $t > 0$, $x, y \in M$. Hence, if $\lambda_1(M) > 0$ then (6.40) provides a correct rate of decay of $p(t, x, y)$ as $t \to \infty$ and as $y \to \infty$.

It turns out that even in the case $\lambda_1(M) = 0$, there is a priori rate of decay of the heat kernel as $t \to \infty$. This is based on the following isoperimetric property of manifolds of bounded geometry.

Theorem 7.7 *Any n-dimensional manifold of bounded geometry admits the following isoperimetric function, for some $c > 0$,*

$$I(v) = c \min\left(v^{\frac{n-1}{n}}, 1\right). \tag{7.29}$$

The meaning of (7.29) is the following. For small v, the function $I(v)$ is nearly the Euclidean one which corresponds to the fact that the small scale geometry of M is uniformly quasi-isometric to that of $\mathbb{R}^n$. For large v, (7.29) gives $I(v) = c$, which is attained on the cylinder $M = \mathbb{R}^{n-1} \times \mathbb{S}^1$ (see Fig. 14). Roughly speaking, (7.29) says that a manifold of bounded geometry expands at ∞ at least as fast as a cylinder.

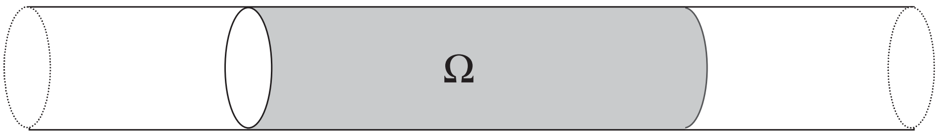

Figure 14 The surface area of $\partial\Omega$ does not increase when the set $\Omega \subset \mathbb{R}^{n-1} \times \mathbb{S}^1$ is stretching.

Proof. We need to show that, for any precompact open set Ω with smooth boundary,

$$\sigma\left(\partial\Omega\right) \geq I(|\Omega|).$$

CASE 1. Assume that, for any $x \in M$, the set Ω covers less than a half of the volume of the ball $B(x, r_0/3)$. Then, for any point $x \in \overline{\Omega}$, there exists a positive number $r(x) \leq r_0/3$ such that

$$\frac{1}{4} \leq \frac{\sigma(\partial\Omega \cap B(x, r(x)))}{V(x, r(x))} \leq \frac{1}{2}. \tag{7.30}$$

All balls $B(x, r(x))$, $x \in \overline{\Omega}$, cover $\overline{\Omega}$. Choose a finite number of them also covering $\overline{\Omega}$. Then, by using the Banach argument, choose out of them a finite family of disjoint balls $B(x_i, r_i)$ (where $r_i = r(x_i)$) so that the concentric balls $B(x_i, 3r_i)$ cover Ω.

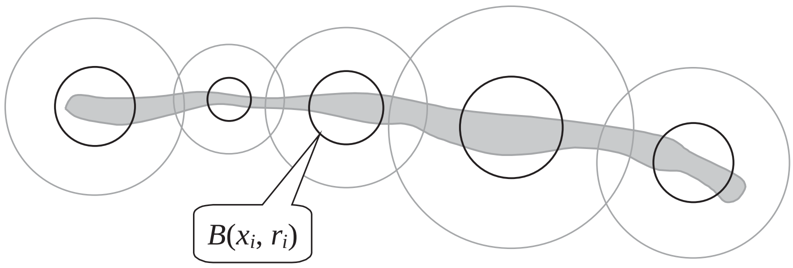

Figure 15 Set Ω (shaded) takes in each ball $B(x_i, r_i)$ nearly one half of its volume, whereas the balls $B(x_i, 3r_i)$ cover all of Ω.

In particular, we have

$$\sum_i V(x_i, 3r_i) \geq |\Omega|\,. \tag{7.31}$$

On the other hand, we use the following isoperimetric property of partitions of balls.

Proposition 7.8 *For any smooth hypersurface Γ in $B(x, r)$ (where $r \leq r_0$) dividing $B(x, r)$ into two open subsets each having volume at least v,*

$$\sigma(\Gamma) \geq c v^{\frac{n-1}{n}}. \tag{7.32}$$

If $B(x, r)$ is a Euclidean ball then (7.32) is a classical inequality, the best constant c in which was found by Maz'ya - see [102]. If $B(x, r)$ is a ball on manifold of bounded geometry and $r \leq r_0$ then (7.32) follows from its Euclidean version and from the fact that the measures of all dimensions in $B(x, r_0)$ differ from their Euclidean counterparts at most by a constant factor.

Applying (7.32) to $\Gamma = \partial\Omega \cap B(x_i, r_i)$ and using (7.30), we obtain

$$\sigma\left(\partial\Omega \cap B(x_i, r_i)\right) \geq c V(x_i, r_i)^{\frac{n-1}{n}}.$$

Adding up these inequalities over all i and applying the elementary inequality

$$\sum_i a_i^{\nu} \geq \left(\sum_i a_i\right)^{\nu}, \tag{7.33}$$

which is valid for $a_i \geq 0$ and $0 \leq \nu \leq 1$, we obtain

$$\sigma(\partial\Omega) \geq c\left(\sum_i V(x_i, r_i)\right)^{\frac{n-1}{n}}. \tag{7.34}$$

Finally, we use $V(x, 3r) \leq CV(x, r)$, which is true for all $r \leq r_0/3$. Therefore, (7.31) and (7.34) imply

$$\sigma(\partial\Omega) \geq c\,|\Omega|^{\frac{n-1}{n}}. \tag{7.35}$$

which was to be proved.

CASE 2. Assume that, for some $x \in M$, the set Ω covers at least a half of the volume of the ball $B(x, r_0/3)$. By moving the point x away, we may assume that

$$|\Omega \cap B(x, r_0/3)| = \frac{1}{2}V(x, r_0/3). \tag{7.36}$$

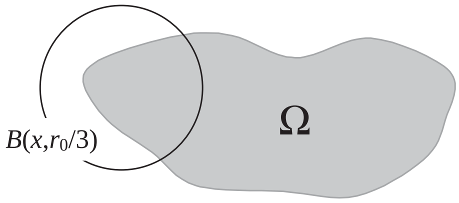

Figure 16 Set Ω covers exactly one half of the volume of the ball $B(x, r_0/3)$.

By Proposition 7.8 and (7.36), we have

$$\sigma(\partial\Omega) \geq \sigma(\partial\Omega \cap B(x, r_0/3)) \geq cV(x, r_0/3)^{\frac{n-1}{n}} \geq \text{const}, \tag{7.37}$$

which together with (7.35) finishes the proof. ■

Theorem 7.7 and Corollary 7.2 imply

Theorem 7.9 *On any manifold of bounded geometry,*

$$p(t, x, x) \leq C\max\left(t^{-n/2}, t^{-1/2}\right),$$

for all $x \in M$ and $t > 0$. In particular, for all $x \in M$ and $t > 1$,

$$p(t, x, x) \leq Ct^{-1/2}. \tag{7.38}$$

The exponent $\frac{1}{2}$ in (7.38) is sharp as is shown by (2.24) for the manifold $M = \mathbb{S}^1 \times \mathbb{R}^{n-1}$. The estimate (7.38) was proved by different methods by Varopoulos [132], Chavel and Feldman [25], Coulhon and Saloff-Coste [39], [34], Grigor'yan [70].

Sharper estimates of the heat kernel can be obtained assuming a *modified* isoperimetric inequality on M. Let us say that M admits a *modified isoperimetric* function $I(v)$ if $\sigma(\partial\Omega) \geq I(|\Omega|)$, for all precompact regions $\Omega \subset M$ with smooth boundary such that Ω contains a ball of the radius r_0. The purpose of this notion introduced by Chavel and Feldman [25] is to separate the large scale isoperimetric properties of the manifold from its local properties. For example, the Riemannian product $M = K \times \mathbb{R}^m$ where K is a compact manifold of the dimension $n - m$, admits the modified isoperimetric function $I(v) = cv^{\frac{m-1}{m}}$ (see [64]). As follows from Theorem 7.7, every manifold of bounded geometry admits the modified isoperimetric function $I(v) = \text{const}$.

Theorem 7.10 *(Chavel – Feldman [25]) If M is a manifold of bounded geometry admitting the modified isoperimetric function $I(v) = cv^{\frac{m-1}{m}}$ then, for all $x \in M$ and $t > 1$,*

$$p(t, x, x) \leq Ct^{-m/2}.$$

Proof. It suffices to verify that M admits the following (not modified!) isoperimetric function

$$v \mapsto c' \begin{cases} v^{\frac{n-1}{n}}, & v \leq 1, \\ v^{\frac{m-1}{m}}, & v \geq 1. \end{cases}$$

The proof of that follows the same line of reasoning as the proof of Theorem 7.7, with the following modification. No change is required for Case 1. In Case 2, take again the point x for which (7.36) is satisfied and consider the region $\Omega_0 = \Omega \cup B(x, r_0)$. Since Ω_0 contains a ball of radius r_0, the modified isoperimetric inequality gives

$$\sigma(\partial\Omega_0) \geq c\, |\Omega_0|^{\frac{m-1}{m}} \geq c\, |\Omega|^{\frac{m-1}{m}}.$$

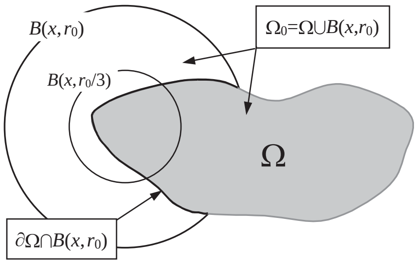

Figure 17 Sets Ω and Ω_0

To finish the proof, it suffices to show

$$\sigma(\partial\Omega_0) \leq C\sigma(\partial\Omega). \tag{7.39}$$

The idea is that by adding the ball to Ω, we do not increase considerably the surface area of $\partial\Omega$ because the part of $\partial\Omega$ covered by the ball is comparable to the boundary of the ball. Formally, we write

$$\begin{aligned} \sigma(\partial\Omega_0) &\leq \sigma(\partial\Omega) + \sigma(\partial B(x, r_0)) \\ &\leq \sigma(\partial\Omega) + Cr_0^{n-1}. \end{aligned} \tag{7.40}$$

On the other hand, as follows from (7.37),

$$\sigma(\partial\Omega \cap B(x, r_0)) \geq cr_0^{n-1}.$$

We see that the first term dominates in (7.40) whence (7.39) follows. ■

See [70] for extension of Theorem 7.10 to a more general setup of manifolds of weak bounded geometry.

The following theorem improves (7.38) assuming the volume growth instead of an isoperimetric inequality.

Theorem 7.11 *(Coulhon – Saloff-Coste [38]) Assume that M has bounded geometry and that*

$$V(x, r) \asymp r^N, \quad \forall x \in M,\ r > 1. \tag{7.41}$$

Then, for all $x \in M$ and $t > 1$,

$$p(t, x, x) \leq Ct^{-\frac{N}{N+1}}. \tag{7.42}$$

Note that $\frac{1}{2} \leq \frac{N}{N+1} < 1$ so that (7.42) is better than (7.38) whenever $N > 1$. The proof of Theorem 7.11 in [38, Theorem 8] contains implicitly the fact that the manifold in question admits the Faber-Krahn function

$$\Lambda(v) = c \begin{cases} v^{-2/n}, & v \leq 1, \\ v^{-\frac{N+1}{N}}, & v \geq 1. \end{cases}$$

Given that much, Theorem 7.11 can be derived from Theorem 6.2. See [35] for further results in this direction.

Let us recall for comparison that Theorem 5.11 yields, under the hypotheses of Theorem 7.11, the following lower bound, for all $x \in M$ and t large enough,

$$p(t,x,x) \geq \frac{c}{(t \log t)^{N/2}}.$$

It seems that the entire range between these two extreme behaviors of the heat kernel given by $t^{-\frac{N}{N+1}}$ and $(t \log t)^{-N/2}$, is actually possible.

Any manifold M of bounded geometry has at most exponential volume growth, that is, for all $x \in M$ and $r > 1$,

$$V(x,r) \leq C \exp(Cr).$$

This follows from the fact that M can be covered by a countable family of balls of radius $r_0/2$, which has a uniformly finite multiplicity (see, for example, [87]). By Theorem 5.13, one obtains the heat kernel lower estimate, for all $x \in M$ and $t \geq t_0,$

$$p(t,x,x) \geq c \exp(-Kt),$$

for some $c > 0$ and $K > 0$. By the chain argument involving the local Harnack inequality, this estimate can be extended to

$$p(t,x,y) \geq c \exp\left(-Kt - C\frac{d^2(x,y)}{t}\right), \tag{7.43}$$

for all $x, y \in M$ and $t \geq t_0$. The difference between (7.28) and (7.43) is that the former is *not* uniform with respect to x. On the other hand, (7.28) provides the sharp rate $e^{-\lambda_1(M)t}$ of the heat kernel decay as $t \to \infty$ whereas the constant K is (7.43) may be much larger than $\lambda_1(M)$ - see [126].

7.6 Covering manifolds

Let Γ be a discrete group of isometries of the manifold M. We say that the manifold M is a *regular cover* of the manifold K with the deck transformation group Γ if K is isometric to the quotient M/Γ. Intuitively, one can imagine M as a manifold glued from many copies of K moving from one to another by using the group action of Γ.

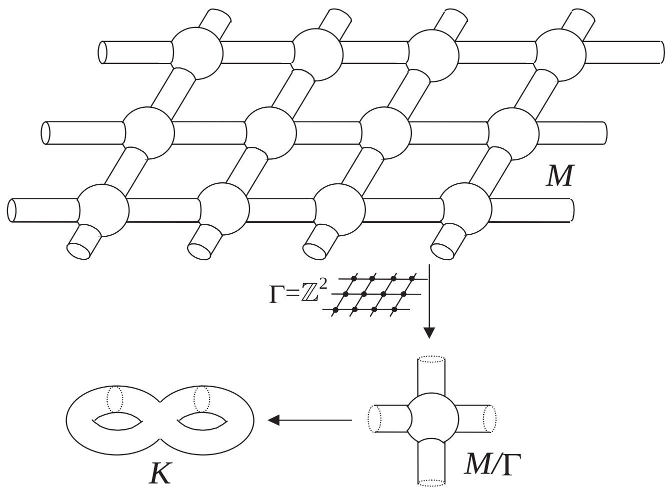

Figure 18 Manifold M covers K by the group $\Gamma = \mathbb{Z}^2$

If M is a regular cover of a compact manifold K then M has bounded geometry so that the results of the previous section apply. However, much more can be said about the heat kernel given the volume growth of M. The following isoperimetric inequality of Coulhon and Saloff-Coste plays the crucial role.

Theorem 7.12 *(Coulhon – Saloff-Coste [38, Theorem 4]) Let a non-compact manifold M be a regular cover of a compact manifold K. Let $\mathcal{V}(r)$ be a positive increasing function on $\mathbb{R}_+$ possessing certain regularity and such that, for some (fixed) $o \in M$ and all $r > 0$,*

$$V(o,r) \geq \mathcal{V}(r). \tag{7.44}$$

Then, for some (large) constant $C > 0$, the manifold M admits the isoperimetric function

$$I(v) := \frac{v}{C\mathcal{V}^{-1}(Cv)}, \tag{7.45}$$

where $\mathcal{V}^{-1}$ is the inverse function.

Next theorem provides the heat kernel upper bound on covering manifolds.

Theorem 7.13 *Referring to Theorem 7.12, we have, for all $x \in M$, $t > 0$ and some $\varepsilon > 0$,*

$$p(t,x,x) \leq \frac{C}{\mathcal{V}(\rho(\varepsilon t))}, \tag{7.46}$$

where ρ is defined by

$$t = \int_0^{\rho(t)} r^2 \frac{d}{dr} \log \mathcal{V}(r)\, dr. \tag{7.47}$$

Proof. Let us apply Corollary 7.2 with the isoperimetric function (7.45). Then the upper bound (7.8) holds with the function f defined by (7.7). Substituting (7.45) into (7.7), we obtain

$$\begin{aligned} t &= 4C^2 \int_0^{f(t)} \frac{\left[\mathcal{V}^{-1}(Cv)\right]^2 dv}{v} \\ &= 4C^2 \int_0^{Cf(t)} \frac{\left[\mathcal{V}^{-1}(v)\right]^2 dv}{v} \\ &= 4C^2 \int_0^{\mathcal{V}^{-1}(Cf(t))} \frac{r^2 d\mathcal{V}(r)}{\mathcal{V}(r)}. \end{aligned}$$

Setting $c = 1/(4C^2)$ and using the definition (7.47) of ρ, we obtain

$$\mathcal{V}^{-1}(Cf(t)) = \rho(ct)$$

and

$$f(t) = C^{-1}\mathcal{V}(\rho(ct)).$$

Hence, (7.46) follows from (7.8). ■

For example, if $V(o,r) \geq cr^N$ then take $\mathcal{V}(r) = cr^N$ and, by (7.47), $\rho(t) \asymp \sqrt{t}$. Hence, (7.46) implies $p(t,x,x) \leq Ct^{-N/2}$.

If $V(o,r) \geq \exp(r^\alpha) =: \mathcal{V}(r)$ (for large r) then we obtain $\rho(t) \asymp t^{\frac{1}{2+\alpha}}$ and

$$p(t,x,x) \leq C \exp\left(-ct^{\frac{\alpha}{2+\alpha}}\right), \tag{7.48}$$

for large t. In the particular case $\alpha = 1$, we have

$$p(t,x,x) \leq C \exp\left(-ct^{1/3}\right). \tag{7.49}$$

It turns out that the exponent $1/3$ here is sharp. Indeed, Alexopoulos [1] showed that a similar on-diagonal lower bound holds provided the deck transformation group Γ is polycyclic and $V(o,r) \asymp \exp(r)$. See [115] for further results of this type.

7.7 Spherically symmetric manifolds

Let us fix the origin $o \in \mathbb{R}^n$, some positive smooth function ψ on $\mathbb{R}_+$ such that

$$\psi(0) = 0 \quad \text{and} \quad \psi'(0) = 1, \tag{7.50}$$

and define a *spherically symmetric* (or *model*) Riemannian manifold M_ψ as follows

1. as a set of points, M_ψ is $\mathbb{R}^n$;
2. in the polar coordinates (r, θ) at o (where $r \in \mathbb{R}_+$ and $\theta \in \mathbb{S}^{n-1}$) the Riemannian metric on $M_\psi \backslash \{o\}$ is defined as
$$ds^2 = dr^2 + \psi^2(r)d\theta^2\,, \tag{7.51}$$
where $d\theta$ denotes the standard Riemannian metric on $\mathbb{S}^{n-1}$;
3. the Riemannian metric at o is a smooth extension of (7.51) possibility of that is ensured by (7.50).

For instance, if $\psi(r) \equiv r$ then (7.51) coincides with the Euclidean metric of $\mathbb{R}^n$ and M_ψ is isometric to $\mathbb{R}^n$. If $\psi(r) = \sinh r$ then M_ψ is isometric to $\mathbb{H}^n$.

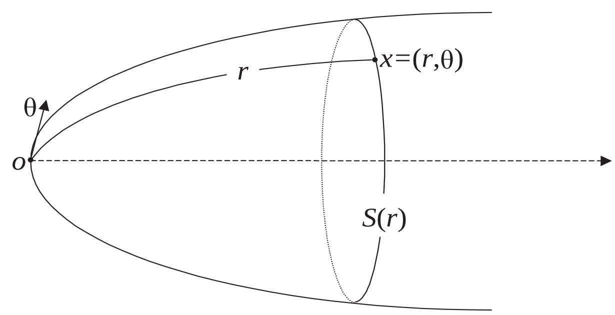

Figure 19 Model manifold as a surface of revolution

Clearly, the surface area $S(r)$ of the geodesic sphere $\partial B(o, r)$ on M_ψ is computed as

$$S(r) = \omega_n \psi^{n-1}(r),$$

and the volume $V(r)$ of the ball $B(o, r)$ is given by

$$V(r) = \int_0^r S(\xi)d\xi = \omega_n \int_0^r \psi^{n-1}(\xi)d\xi.$$

The Laplace operator on M_ψ can be written as follows (see [63], [122, p.97])

$$\Delta = \frac{\partial^2}{\partial^2 r} + \frac{S'}{S}\frac{\partial}{\partial r} + \frac{1}{\psi^2}\Delta_\theta\,, \tag{7.52}$$

where Δ_θ denotes the Laplace operator on the sphere $\mathbb{S}^{n-1}$.

We would like to estimate the heat kernel $p(t, x, x)$ on M_ψ by using Corollary 7.2. Isoperimetric function $I(v)$ seems to be unknown for general ψ. However, if we restrict our talk to estimating $p(t, o, o)$ then there is a simple way out. Careful analysis of the proof of Corollary 7.2 shows that we need to know the isoperimetric inequality

$$\sigma(\partial\Omega) \geq I(|\Omega|) \tag{7.53}$$

only for those sets Ω which are level sets of the function $p(t, o, \cdot)$, that is, for the two-parameter family of regions

$$\Omega_{s,t} = \{x \in M : p(t, o, x) > s\}$$

(see [36, Proposition 8.1]).

Given the rotation symmetry of M_ψ with respect to the point o, it is easy to prove that all $\Omega_{s,t}$ are ball centered at o. Hence, we need to find the function I such that (7.53) holds for all balls $\Omega = B(o, r)$. Since there is only one ball $B(o, r)$ with a prescribed volume, the isoperimetric function I can be defined by

$$I(v) = S(r) \quad \text{if } V(r) = v.$$

In order to apply Corollary 7.2, $I(v)/v$ should be non-increasing which amounts to the non-increasing of $S(r)/V(r)$. The equation (7.7) for $f(t)$ becomes

$$t = 4 \int_0^{V^{-1}(f(t))} \frac{V(r)dr}{S(r)}.$$

Hence, we arrive to the following conclusion.

Theorem 7.14 *([36, Theorem 8.3]) Suppose that, for a model manifold M_ψ, the function $S(r)/V(r)$ is non-increasing. Let us define the function $\rho(t)$ by*

$$t = 4 \int_0^{\rho(t)} \frac{dr}{\frac{d}{dr} \log V(r)}. \tag{7.54}$$

Then, for all $t > 0$ and $\varepsilon \in (0, 1)$,

$$p(t, o, o) \leq \frac{C_\varepsilon}{V(\rho(\varepsilon t))}. \tag{7.55}$$

For example, if $V(r) = Cr^N$ then (7.54) gives $\rho(t) \asymp \sqrt{t}$ and (7.55) implies

$$p(t, o, o) \leq \frac{C'}{V(\sqrt{t})} = \frac{C''}{t^{N/2}}.$$

Note that, by Theorem 5.12, we have in this case the matching lower bound for $p(t, o, o)$. More generally, if $V(r)$ is doubling (see (5.38)) then one obtains from Theorems 7.14 and 5.12

$$p(t, o, o) \asymp \frac{1}{V(\sqrt{t})}$$

(see [36, Corollary 8.5]).

If $V(r) = \exp(r^\alpha)$, $0 < \alpha \leq 1$, then we obtain $\rho(t) \asymp t^{\frac{1}{2-\alpha}}$ and

$$p(t, o, o) \leq C \exp\left(-ct^{\frac{\alpha}{2-\alpha}}\right). \tag{7.56}$$

Theorem 5.13 yields for this volume growth the matching lower bound - cf. (5.42).

It is interesting that, for covering manifold M with the same volume growth function, the upper bound (7.48) is *weaker* than (7.56). In some sense, model manifolds possess the smallest heat kernel per volume growth function. This happens because all directions from o to the infinity are equivalent, which maximizes the capability of the Brownian motion to escape to the infinity and, thereby, minimizes the heat kernel $p(t, o, o)$. On covering manifolds, there may exists two non-equivalent ways of escaping (this is the case, for example, if the desk transformation group Γ is polycyclic) one of them being "narrow" in some sense and providing for a higher probability of return.

7.8 Manifolds of non-negative Ricci curvature

The main result of this section is the following isoperimetric inequality on non-negatively curved manifolds.

Theorem 7.15 *Let M be a geodesically complete non-compact Riemannian manifold of non-negative Ricci curvature. Then, for any ball $B(z,R) \subset M$ and any open set $\Omega \subset B(z,R)$ with smooth boundary,*

$$\frac{\sigma(\partial\Omega)}{|\Omega|} \geq \frac{c}{R}\left(\frac{V(z,R)}{|\Omega|}\right)^{1/n} \tag{7.57}$$

where $n = \dim M$ and $c = c(n) > 0$.

By Proposition 7.1, the isoperimetric inequality (7.57) implies the relative Faber-Krahn inequality (6.42) (the latter was proved for manifolds of non-negative Ricci curvature in [67]). Hence, Theorems 6.13 and 5.9 imply the following upper bound of the heat kernel on M

$$p(t,x,y) \leq \frac{C}{\sqrt{V(x,\sqrt{t})V(y,\sqrt{t})}} \exp\left(-\frac{d^2(x,y)}{2Dt}\right), \tag{7.58}$$

where $D > 2$. This estimate was first obtained by Li and Yau [98]. They also proved the matching lower bound

$$p(t,x,y) \geq \frac{c}{\sqrt{V(x,\sqrt{t})V(y,\sqrt{t})}} \exp\left(-\frac{d^2(x,y)}{2Dt}\right), \tag{7.59}$$

for $D < 2$. Some improvements of these estimates can be found in [93]. See [134], [46] for heat kernel estimates on manifolds with $Ric_M \geq -K$, and [81] for similar heat kernel estimates in unbounded regions in $\mathbb{R}^n$ with the Neumann boundary condition.

We precede the proof of (7.57) by two properties of non-negatively curved manifolds.

Lemma 7.16 *Let M be a geodesically complete non-compact manifold of non-negative Ricci curvature. Then, for all balls intersecting $B(x,r)$ and $B(y,r')$ with $r \leq r'$,*

$$c\left(\frac{r'}{r}\right)^{\varepsilon} \leq \frac{V(y,r')}{V(x,r)} \leq C\left(\frac{r'}{r}\right)^{n}, \tag{7.60}$$

where ε, c, C are positive and depend on n.

Proof. We use Gromov's volume comparison theorem which says that if $Ric_M \geq 0$ then, for all $x \in M$ and $r' \geq r > 0$,

$$\frac{V(x,r')}{V(x,r)} \leq \left(\frac{r'}{r}\right)^{n} \tag{7.61}$$

(see [27], [23], [22]).

Denote $\delta = d(x,y)$. Then $\delta \leq r' + r \leq 2r'$, and the right hand inequality in (7.60) follows by (7.61)

$$\frac{V(y,r')}{V(x,r)} \leq \frac{V(x,r'+\delta)}{V(x,r)} \leq \left(\frac{r'+\delta}{r}\right)^{n} \leq \left(\frac{3r'}{r}\right)^{n} = 3^n\left(\frac{r'}{r}\right)^{n}.$$

To prove the left hand inequality in (7.60), let us first verify it in the particular case $r' = 3r$ and $y = x$. Find a point ξ such that $d(x,\xi) = 2r$ (here we use the completeness and non-compactness of M). Then $B(\xi,r)$ is contained in $B(x,3r)$ but does not intersect $B(x,r)$. Hence, we obtain

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

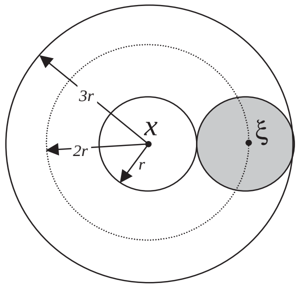

Figure 20 Ball $B(\xi,r)$ is contained in $B(x,3r)$ but does not intersect $B(x,r)$

In general, let us find an integer k such that

$$3^k \le \frac{r'}{r} < 3^{k+1}.$$

Then

$$V(y,r') \ge C^{-1}V(x,r') \ge C^{-1}V(x,3^k r) \ge C^{-1}(1+C^{-1})^k V(x,r)$$

and

$$\frac{V(y,r')}{V(x,r)} \ge C^{-1}\left(1+C^{-1}\right)^k \ge c\left(\frac{r'}{r}\right)^{\log_3\left(1+C^{-1}\right)},$$

which was to be proved. ■

Lemma 7.17 *(Buser [18]) Let M be a geodesically complete manifold of non-negative Ricci curvature. Then, for any ball $B(x,r)$ and for any smooth hypersurface Γ in $B(x,r)$ dividing $B(x,r)$ into two sets both having volume at least v,*

$$\sigma(\Gamma) \ge c\frac{v}{r}, \tag{7.62}$$

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

Observe that inequality (7.62) follows from (7.32) if $M = \mathbb{R}^n$. We refer the reader to [18, Lemma 5.1] or [67, Theorem 2.1] for the proof in general case.

Proof of Theorem 7.15. The proof is similar to Theorem 7.7. For any point $x \in \Omega$, let us find a positive $r(x)$ so that Ω covers exactly one half of the volume of $B(x, r(x))$. To that end, consider the function

$$h(r) := \frac{|\Omega \cap B(x,r)|}{V(x,r)}.$$

For r small enough, we have $h(r) = 1$. If $r > R$ then, by Lemma 7.16,

$$h(r) \le \frac{|\Omega|}{V(x,r)} \le \frac{V(z,R)}{V(x,r)} \le c^{-1}\left(\frac{R}{r}\right)^{\varepsilon}.$$

In particular, if the ratio r/R is large enough then $h(r) < 1/2$. Hence, for some $r \le C'R$, we have $h(r) = 1/2$.

The family of balls $B(x, r(x))$, $x \in \Omega$, covers Ω. By using the Banach ball covering argument, we can select at most countable subset $B(x_i, r_i)$ (where $r_i = r(x_i)$) so that the balls $B(x_i, r_i)$ are disjoint whereas the union of $B(x_i, 5r_i)$ covers Ω. The latter implies

$$\sum_i V(x_i, r_i) \ge 5^{-n}\sum_i V(x_i, 5r_i) \ge 5^{-n}|\Omega|. \tag{7.63}$$

On the other hand, Lemma 7.17 and the fact that

$$|\Omega \cap B(x_i, r_i)| = \frac{1}{2}V(x_i, r_i),$$

imply

$$\sigma(\partial\Omega \cap B(x_i, r_i)) \ge \frac{c}{2r_i}V(x_i, r_i). \tag{7.64}$$

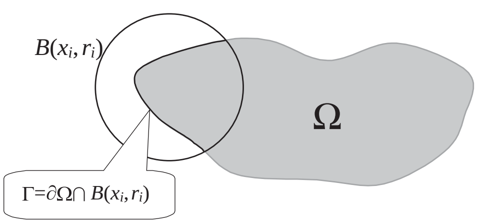

Figure 21 Estimating the area of Γ via the volumes of the sets $\Omega \cap B(x_i, r_i)$ and $B(x_i, r_i) \setminus \Omega$

Since
$$\frac{V(z,R)}{V(x,r_i)} \leq \frac{V(x,R+r_i)}{V(x,r_i)} \leq \frac{V(x,R(1+C'))}{V(x,r_i)} \leq C'' \left(\frac{R}{r_i}\right)^n,$$
we have
$$\frac{1}{r_i} \geq \frac{c'}{R}\left(\frac{V(z,R)}{V(x,r_i)}\right)^{1/n}.$$
By substituting into (7.64), we obtain
$$\sigma\left(\partial\Omega \cap B(x_i,r_i)\right) \geq \frac{c'}{R} V(z,R)^{1/n} V(x_i,r_i)^{1-1/n}.$$
Finally, summing up over all i and applying (7.33) and (7.63), we conclude
$$\sigma\left(\partial\Omega\right) \geq \frac{c''}{R} V(z,R)^{1/n} \left|\Omega\right|^{1-1/n},$$
which is equivalent to (7.57). ■

By Corollary 6.14, the upper bound (7.58) is equivalent to the relative Faber-Krahn inequality, under the standing assumption of the doubling volume property. It turns out that the conjunction of both upper and lower bounds (7.58) and (7.59) is equivalent to *the Poincaré inequality*
$$\int_{B(x,2r)} |\nabla f|^2 \, d\mu \geq \frac{c}{r^2} \inf_{\xi\in\mathbb{R}} \int_{B(x,r)} (f-\xi)^2 \, d\mu, \tag{7.65}$$
which is meant to hold for all $x \in M$, $r > 0$ and $f \in C^1(B(x,2r))$ (see [67], [68], [120], [121]). One can regard (7.65) as the L^2-version of the isoperimetric inequality (7.62). Indeed, the later is equivalent to the functional inequality
$$\int_{B(x,2r)} |\nabla f| \, d\mu \geq \frac{c}{r^2} \inf_{\xi\in\mathbb{R}} \int_{B(x,r)} |f-\xi| \, d\mu. \tag{7.66}$$
Theorem 7.15 can be stated as the implication (7.66)⇒(7.57). Similarly, one can prove that (7.65) implies the relative Faber-Krahn inequality (6.42) - see [67, Theorem 1.4] and [120, Theorem 2.1].

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