The heat kernel and its estimates

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Abstract.

After a short survey of some of the reasons that make the heat kernel an important object of study, we review a number of basic heat kernel estimates. We then describe recent results concerning (a) the heat kernel on certain manifolds with ends, and (b) the heat kernel with the Neumann or Dirichlet boundary condition in inner uniform Euclidean domains.

§1.   Introduction

This text is a revised version of the four lectures given by the author at the First MSJ-SI in Kyoto during the summer of 2008. The structure of the lectures has been mostly preserved although some material has been added, deleted, or shifted around. The goal is to present an overview of the study of the heat kernel, in the context of the theme of the meeting, that is, "Probabilistic Approach to Geometry". There is certainly ample evidence that the study of the heat kernel is an area of fruitful interactions between the fields of Analysis, Probability and Geometry and this will be illustrated here again. The simplest statement embodying these interactions is perhaps Varadhan's large deviation formula [60]

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

This formula relates the heat kernel $p(t, x, y)$ to the Riemannian distance function $d(x, y)$ on a complete Riemannian manifold. A remarkable generalization was given by Hino and Ramirez (see, [3, 39]). Namely, in the context of Dirichlet spaces,

$$\lim_{t \to 0} -4t \log \mathbb{P}(X_0 \in A; X_t \in B) = d(A, B)^2.$$

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Here X_t denotes the Markov process associated with the underlying local regular Dirichlet form and d is the associated intrinsic distance. Unfortunately, these elegant statements are not very easy to use in practice. They do capture the essence of the universal Gaussian character of the heat kernel but they are quite far from providing upper and/or lower bounds comparing the heat kernel $p(t, x, y)$ to expressions of the form

$$(1) \qquad\qquad F(t, x, y) \exp\left(-\frac{d(x, y)^2}{ct}\right),$$

where $F(t, x, y)$ is some explicit function whose role is to describe the behavior of the heat kernel in the region where $d(x, y)^2 \le t$. Of course, in the classical case of the n-dimensional Euclidean space $\mathbb{R}^n$, $F(t, x, y)$ is simply a function of t and

$$(2) \qquad p(t, x, y) = \left(\frac{1}{4\pi t}\right)^{n/2} \exp\left(-\frac{d(x, y)^2}{4t}\right), \ t > 0, \ x, y \in \mathbb{R}^n.$$

Upper and lower bounds of the type (1) are the focus of this article. After discussing in Lecture 1 some general upper bounds and their relations to functional inequalities, we will survey a number of results that provide (almost) matching heat kernel upper and lower bounds. The most important of these results is described in Lecture 2 and characterizes those complete Riemannian manifolds on which the heat kernel is bounded by

$$(3) \qquad\qquad p(t, x, y) \simeq \frac{1}{V(x, \sqrt{t})} \exp\left(-\frac{d(x, y)^2}{t}\right),$$

by which we means that there are constants $c_i \in (0, \infty)$ such that

$$\frac{c_1}{V(x, \sqrt{t})} \exp\left(-\frac{d(x, y)^2}{c_2 t}\right) \le p(t, x, y) \le \frac{c_3}{V(x, \sqrt{t})} \exp\left(-\frac{d(x, y)^2}{c_4 t}\right).$$

In Lecture 3, this fundamental result is used to study a large class of manifolds with finitely many ends where (3) does not hold but where the function F in (1) can nevertheless be described explicitly in reasonably simple geometric terms. Finally, in Lecture 4, the characterization of (3) discussed in Lecture 2 is applied to the study of the heat kernel with Dirichlet boundary condition in some Euclidean domains.

§**2. Lecture 1: Motivations and basic heat kernel bounds**

We let M denote our generic underlying space. It is, at the very least, a topological (metrizable, locally compact) space equipped with

a measure $\mu(dy) = dy$ and a "Laplacian" Δ. The reader can think of a complete non-compact Riemannian manifold equipped with the Riemannian measure $v(dy)$ and the Laplacian $\Delta = \text{div grad}$ as the basic example. But the reader should also keep in mind that we will want to include further examples, the simplest of which are weighted Riemannian manifolds, that is, complete non-compact Riemannian manifolds equipped with a measure $\mu(dy) = \sigma(y)v(dy)$, $0 < \sigma \in \mathcal{C}^\infty(M)$, and the associated weighted Laplacian $\Delta = \sigma^{-1}\text{div}(\sigma\text{grad})$.

Of course, the most classical case is $M = \mathbb{R}^n$ equipped with Lebesgue measure and $\Delta = \sum_1^n \left(\frac{\partial}{\partial x_i}\right)^2$. In this case the heat kernel $p(t, x, y)$ is given by (2).

2.1.   What is the heat kernel?

There are many ways to introduce the heat kernel and each has its own advantages. Let us mention three distinct viewpoints.

The first is to view the heat kernel as the fundamental solution of a parabolic partial differential equation, the heat diffusion equation

$$(4) \qquad\qquad (\partial_t - \Delta)u = 0.$$

That is, we seek a smooth function $(t, x, y) \mapsto p(t, x, y)$ defined on $(0, \infty) \times M \times M$ such that, for each $y \in M$, $p(t, x, y)$ is a solution of (4) and for any $\phi \in \mathcal{C}_c^\infty(M)$ (smooth compactly supported function on M), $u(t, x) = \int_M p(t, x, y)\phi(y)dy$ tends to $\phi(x)$ as t tends to 0. In other words, the heat kernel allows us to solve the Cauchy initial value problem for (4).

A second possibility is to consider Δ (defined, say, on $\mathcal{C}_c^\infty(M)$) as a symmetric operator on $L^2(M, \mu)$ whose Friederichs extension generates a strongly continuous one parameter contraction semigroup H_t on $L^2(M, \mu)$ (the heat diffusion semigroup). This semigroup admits a transition function (a priori, this is a measure in the second variable) $p(t, x, dy)$ such that $H_t f(x) = \int_M f(y)p(t, x, dy)$. The heat kernel (if it exists) is then obtained as the density of $p(t, x, dy)$ with respect to the underlying measure $\mu(dy) = dy$.

A third approach is to view $p(t, x, dy)$ as the distribution at time t of a stochastic process $(X_t)_{t>0}$ started at x (the Brownian motion driven by Δ on M). These different viewpoints are related by the formula

$$u(t, x) = H_t u_0(x) = \mathbb{E}_x(u_0(X_t))$$

where u is the solution of the Cauchy initial value problem for (4) with initial value condition u_0 (say, in $\mathcal{C}_c^\infty(M)$).

2.2.   Why is this interesting or useful?

2.2.1. *Intrinsic interest* The study of the parabolic equation (4) is justified by its dual interpretation as the equation modeling heat diffusion and the equation driving Brownian motion. Estimating the heat kernel is to understand the space-time evolution of temperature in an object represented by M. From this view point, one may want to study:

- the long time behavior of the maximal temperature $\phi(t) = \sup_{x,y\in M}\{p(t,x,y)\}$;
- the long time behavior of the maximal temperature for a fixed starting point x, $\phi(t,x) = \sup_{y\in M} p(t,x,y)$;
- the long time behavior of the temperature at a fixed point y for a fixed starting point x, i.e., the behavior of $p(t,x,y)$.
- the evolution of the position and shape of the hot spot set (for some fixed $\epsilon \in (0,1)$)

$$\mathrm{HOT}_\epsilon(t,x) = \{y \in M : p(t,x,y) \geq \epsilon\phi(t,x)\}.$$

Obviously, in Euclidean space, (2) indicates that

$$\phi(t) = \phi(t,x) = p(t,x,x) = (4\pi t)^{-n/2}$$

and

$$\mathrm{HOT}_\epsilon(t,x) = B(x, \sqrt{4t\log 1/\epsilon}).$$

This should be compared to what happens in Hyperbolic 3-space where

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

so that $\phi(t) = \phi(t,x) = p(t,x,x) = (4\pi t)^{-3/2}e^{-t}$ and, for all $t > 0$, $\mathrm{HOT}_\epsilon(t,x)$ is contained in $B(x,r(\epsilon))$, a ball whose radius is independent of t. This illustrates the important fact that the behavior of heat kernel is influenced by and captures certain geometric properties of the underlying space.

2.2.2. *The heat kernel as an analytic tool* One of the most basic application of the heat kernel (and the associated heat semigroup) is as a smoothing approximation tool, taking advantage of the fundamental property that $H_t f \to f$ as t tends to 0, under various circumstances. In fact, and this is very useful, many function spaces can be characterized in terms of the behavior of $H_t f$. For instance, the space $\Lambda_\alpha(\mathbb{R}^n)$ of all bounded Hölder continuous functions of exponent $\alpha \in (0,1)$ can be characterized as ($H_t' f$ denotes the time derivative of $H_t f$)

$$\Lambda_\alpha = \{f \in L^\infty(\mathbb{R}^n) : \sup_{t>0}\{t^{1-\alpha/2}\|H_t' f\|_\infty\} < \infty\}.$$

Similarly, one of the equivalent definition of the Hardy space H_1 (whose dual is BMO), is that

$$H_1 = \{f \in L^1(\mathbb{R}^n) : \sup_{t>0} |H_t f| \in L^1(\mathbb{R}^n)\}.$$

See, e.g., [12] and [59, Chapter I]. The whole scales of Besov and Lizorkin spaces can be treated in similar ways. One of the point we want to make here is that these versions of the definitions of classical function spaces are suitable for extensions to a great variety of different setups when other approaches may not be available. In such cases, heat kernel estimates become essential to understand the meaning of these definitions.

Another important application of heat kernel bounds concerns operators that are defined through functional calculus in terms of the Laplacian. For instance, the basic spectral theory of selfadjoint operators allows us to make sense of the operator (often called a multiplier) $m(-\Delta) = \int_0^\infty m(\lambda)dE_\lambda$ acting on L^2 whenever $m : [0,\infty) \to \mathbb{R}$ is bounded continuous. Here, the E_λ's are orthogonal projections that form a spectral resolution of the Laplacian on $L^2(M,\mu)$. To obtain more information on such operators — e.g., does $m(-\Delta)$ also act on L^p for some $p \in (1,\infty)$? — one needs to understand better the spectral projection operators E_λ. Understanding the heat kernel is a very efficient way to study this question since, formally, $p(t,x,y) = \int_0^\infty e^{-t\lambda}dE_\lambda(\delta_x, \delta_y)$ where δ_x denotes the Dirac mass at x. In some sense, $p(t,x,y)$ can serve as an approximation for the spectral projectors E_λ. The simplest application of this general line of thought leads to the resolvent function formula (where $G_\alpha(x,y)$ is the kernel of $(\alpha I - \Delta)^{-1}$, if it exists)

$$G_\alpha(x,y) = \int_0^\infty e^{-\alpha t} p(t,x,y)dt, \quad \alpha \geq 0.$$

A more sophisticated applications concerns the action of the imaginary power of the Laplacian $(-\Delta)^{i\beta}$ on the L^p spaces. See, e.g., [24]. In a similar spirit, heat kernel bounds play a crucial role in the study of the boundedness of Riesz transforms on L^p spaces on manifolds. See [7] and Hofmann article in [40]. Finally, the complex time heat kernel and heat semigroup can also be investigated. See, e.g., [21]. This plays an important role in connection with the study of the multipliers mentioned above and of the wave equation.

2.2.3. *Applications to Topology/Geometry* It is well known that topological/geometrical information is contained in the spectrum of the Laplacian. The heat kernel is a useful tool to extract such information (see, e.g., [40]). This can be done both through asymptotic expansion as t

tends to 0 and through the large time behavior of the heat kernel. For instance, topological dimension and volume growth are reflected in various ways in heat kernel behaviors. In this spirit, more sophisticated properties such as isoperimetric inequalities are also relevant.

2.2.4. *Gaussian Hilbert spaces* One of the most important stochastic process, beside Brownian motion, is the Orstein-Ulhenbeck process. Classically, this is the process on $\mathbb{R}$ associated with the Dirichlet form $\int |f'|^2 d\gamma$ on $L^2(\mathbb{R}, \gamma)$ where γ is Gauss measure. It is one of the basic object of Mathematical Physics. Hermite polynomials provide an orthonormal basis for $L^2(\mathbb{R}, \gamma)$ and diagonalize the associated infinitesimal generator. The heat kernel measure $\mu_t^x(dy) = p(t, x, y)dy$ (with base point x) allows us to define the Gaussian Hilbert space $L^2(M, \mu_t^x)$ in many different settings. These Hilbert spaces are the building blocks of analysis on paths and loop spaces. See. e.g., Driver article in [8] and [35]. Of course, heat kernel estimates are crucial to our understanding of these objects.

2.3.   Sobolev-type inequalities and basic heat kernel bounds

To fix ideas, we frame the following discussion in the context of weighted Riemannian manifolds. Throughout this section, we let (M, g) be a complete non-compact Riemannian manifold equipped with a smooth positive weight σ and the measure $\mu(dy) = \sigma(y)dy$ where dy stands for the Riemannian measure. The associated Laplacian is

$$\Delta f = \sigma^{-1} \mathrm{div}(\sigma \ \mathrm{grad} f).$$

This operator, defined on $\mathcal{C}_c^\infty(M)$ is essentially selfadjoint on $L^2(M, \mu)$ with unique selfadjoint extension $\overline{\Delta}$. We let $p(t, x, y)$ be the associated heat kernel, i.e., the kernel associated to the heat semigroup $e^{t\overline{\Delta}}$ on $L^2(M, \mu)$.

2.3.1. *Varopoulos' theorem* Although there are various antecedents in the literature, N. Varopoulos [61] was the first to identify the equivalence between heat kernel bounds and Sobolev inequality in a large enough context. In particular, Varopoulos proved, for any fixed $n > 2$, the equivalence between the heat kernel upper bound

$$(5) \qquad \phi(t) = \sup_{x,y}\{p(t, x, y)\} \le Ct^{-n/2}, \ \ t > 0,$$

and the Sobolev inequality

$$(6) \qquad \|f\|_{2n/(n-2)}^2 \le S \int_M |\nabla f|^2 d\mu, \ \ f \in \mathcal{C}_c^\infty(M).$$

Other developments in this direction are recorded in the following theorem. See, e.g., [13, 27, 42, 48, 51, 53, 63].

Theorem 2.1. *For any fixed $n > 0$, the bound* (5) *is equivalent to each the following properties:*

- *The Nash inequality:*

$$\forall f \in \mathcal{C}_c^\infty(M), \;\; \|f\|_2^{2(1+2/n)} \leq N \left(\int |\nabla f|^2 d\mu \right) \|f\|_1^{4/n}.$$

- *The Faber-Krahn inequality*

$$\lambda(\Omega) \geq c\mu(\Omega)^{-2/n}$$

   for all open relatively compact subsets Ω of M where $\lambda(\Omega)$ is the lowest Dirichlet eigenvalue in Ω.

Moreover, when $n > 2$, is also equivalent to:

- *The Sobolev inequality* (6).
- *The Rozenblum-Cwikel-Lieb inequality:*

$$\mathcal{N}_-(-\Delta + V) \leq K \int V_-^{n/2} d\mu$$

   where V_- is the negative part of $V \in L_{\mathrm{loc}}^1$ and $\mathcal{N}_-(A)$ is the number of negative L^2-eigenvalues of A.

Note that the lowest Dirichlet eigenvalue in a open set Ω is defined by the variational formula

$$\lambda(\Omega) = \inf \left\{ \frac{\int |\nabla \phi|^2 d\mu}{\int |\phi|^2 d\mu} : \phi \in \mathcal{C}_c^\infty(\Omega), \phi \neq 0 \right\}.$$

See, e.g., [14, 27]. For a topological application of the RCL inequality, see [15].

2.3.2. *The general Gaussian upper bound* One of the most important discovery in the area of heat kernel estimates is the "universality" of the Gaussian factor.

This is illustrated by the following result due to A. Grigor'yan which is typical of an important body of work developed by E.B. Davies, N. Varopoulos, A. Grigor'yan and others concerning Gaussian bounds. See [13, 17, 22, 27, 28, 51, 63]. Given a continuous decreasing function v, we consider the condition

$$(*) \qquad \exists \, 0 < a < 1 < A < \infty, \;\; u(As) > au(s), \;\; u = v'/v.$$

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This condition means that the logarithmic derivative u of v decays at most as a power function in the sense that $u(s)/u(t) \geq c(t/s)^\gamma$ for all $s > t > 0$ and some $c, \gamma > 0$.

Theorem 2.2. *Let v be a continuously differentiable decreasing positive function on $(0, \infty)$ satisfying (*). Let Λ be the continuous function related to v by*

$$t = \int_0^{v(t)} \frac{ds}{s\Lambda(s)}$$

equivalently, $v'(t) = v(t)\Lambda(v(t))$, $v(0) = 0$. Then the Faber-Krahn inequality

$$\lambda(\Omega) \geq c_1\Lambda(C_1\mu(\Omega)), \quad \Omega \text{ open relatively compact in } M,$$

is equivalent to the heat kernel bound

$$\phi(t) = \sup_{x,y}\{p(t,x,y)\} \leq \frac{C_2}{v(c_2 t)}, \quad t > 0.$$

Moreover, these equivalent properties imply

$$\left|\left(\frac{\partial}{\partial t}\right)^m p(t,x,y)\right| \leq \frac{C(m,\epsilon)}{t^m v(ct)} \exp\left(-\frac{d(x,y)^2}{4(1+\epsilon)t}\right),$$

for all $(t, x, y) \in (0, \infty) \times M \times M$.

2.4. Volume growth and heat kernel bounds

One of the most basic ideas relating heat kernel estimates and geometry is that, because of the diffusive character of the heat equation, large volume growth should implies that the heat kernel is small. Here volume growth refers to the volume function $V(x,r) = \mu(B(x,r))$. We now state one of the simplest result illustrating this idea (and its shortcomings). We say that a weighted manifold has bounded geometry if (a) (M, g) satisfies Ric $\geq -kg$ for some $k \geq 0$; (b) $c_1 \leq \sigma(x)/\sigma(y) \leq C_1$ for all x, y with $d(x, y) \leq 2$; (c) $c_1 \leq V(x, 1) \leq C_1$. Under these conditions, the heat kernel satisfies

$$c_2 \leq t^{n/2}p(t,x,x) \leq C_2, \quad (t,x) \in (0,1) \times M,$$

where n is the topological dimension of M.

Theorem 2.3. *Let M be a complete non-compact weighted manifold with bounded geometry (as defined above).*

- *Assume that $V(x, r) \geq cr^N$ for all $r \geq 1$. Then*

$$p(t, x, y) \leq \frac{C}{t^{N/(N+1)}}, \quad t \geq 1.$$

- *Assume that $V(x, r) \leq Cr^N$ for all $r \geq 1$. Then*

$$p(t, x, x) \geq \frac{c}{(t \log t)^{N/2}}, \quad t \geq 1.$$

These bounds are (essentially) sharp in the sense that there are examples where they describe (essentially) the true behavior of the heat kernel. See [9, 18, 19] for details.

The following result complement the previous theorem by giving an important collection of examples where the long time behavior of the heat kernel is tightly connected to the volume growth. Let $M = G$ be a connected unimodular Lie group equipped with Haar measure and a left-invariant Riemannian metric. Let $V(r)$ be the volume of a ball of radius r. Then either (a) there exists D such that $V(r) \simeq r^D$, $r \in (1, \infty)$, or (b) $\log V(r) \simeq r$, $r \in (1, \infty)$. See [63] for details and references for this classical result.

Theorem 2.4. *Let $M = G$ be a connected amenable unimodular Lie group equipped with Haar measure and a left-invariant Riemannian metric. Let $V(r)$ be the volume of a ball of radius r. Then:*

- *Either there exists D such that $V(r) \simeq r^D$, $r \in (1, \infty)$, and the heat kernel satisfies $p(t, x, y) \simeq t^{-D/2}$, $t \in (1, \infty)$.*
- *Or $\log V(r) \simeq r$, $r \in (1, \infty)$, and the heat kernel satisfies $-\log(p(t, x, y)) \simeq t^{1/3}$, $t \in (1, \infty)$).*

See also [52, 53] for a further review of results in this direction and references. The second case, i.e., for amenable unimodular connected Lie groups of exponential volume growth, the estimate take the form

$$\exp\left(-c_1 t^{1/3}\right) \leq p(t, x, x) \leq \exp\left(-C_1 t^{1/3}\right), \quad x \in G, \ t \geq C_2,$$

for some $c_1, C_1, C_2 \in (0, \infty)$.

§3.   Lecture II: The parabolic Harnack inequality (PHI)

3.1.   Harnack inequalities

3.1.1. *The elliptic Harnack inequality* One of the classical result concerning harmonic functions in $\mathbb{R}^n$ states that any positive harmonic

function u in an Euclidean ball $B = B(x, r)$ satisfies

$$(7) \qquad \sup_{(1/2)B}\{u\} \leq H \inf_{(1/2)B}\{u\}.$$

The constant H is independent of B (location and scale) and u. This is known as the (elliptic) Harnack inequality. Its best known consequence is the fact that global positive harmonic functions in $\mathbb{R}^n$ must be constant.

J. Moser [44] observed that (7) also holds for uniformly elliptic operators (with measurable coefficients) in divergence form in $\mathbb{R}^n$ and that this implies the crucial Hölder continuity property of the local solutions of the associated elliptic equation, a result proved earlier by De Giorgi.

In the context of weighted Riemannian manifolds, we may consider the above elliptic Harnack inequality as a property that may or may not be satisfied. It is an open question to characterize (in useful terms) those weighted manifolds that satisfy this property. However, around 1975, Cheng and Yau [16] proved that on any complete Riemannian manifold (M, g) with Ricci curvature bounded below by $\text{Ric} \geq -Kg$, for some $K \geq 0$, any positive harmonic function in a ball $B = B(x, r)$ satisfies

$$|\nabla \log u| \leq C(n)(K + 1/r) \text{ in } (1/2)B.$$

When $K = 0$ (non-negative Ricci curvature), this gradient Harnack estimate immediately implies the validity of (7).

3.1.2. *The parabolic Harnack inequality (PHI)* The parabolic version of (7) is attributed by J. Moser to Hadamard and Pini. In [45], J. Moser proved the parabolic Harnack inequality for uniformly elliptic operators in divergence form in $\mathbb{R}^n$. This inequality states that a positive solution u of the heat equation in a cylinder of the form $Q = (s, s + \alpha r^2) \times B(x, r)$ satisfies
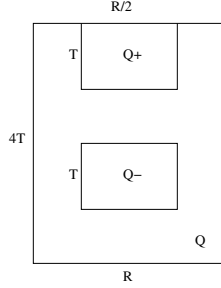
$$(8) \qquad \sup_{Q_-}\{u\} \leq H_0 \inf_{Q_+}\{u\}$$

where, for some fixed $0 < \beta < \gamma < \sigma < \alpha < \infty$ and $\eta \in (0, 1)$,

$$Q_- = (s + \beta r^2, s + \gamma r^2) \times B(x, \eta r), \quad Q_+ = (s + \sigma r^2, s + \alpha r^2) \times B(x, \eta r).$$

Here the constant H_0 is independent of x, r and u. The geometry of the cylinders $Q_-, Q_+ \subset Q$ is depicted in Figure 1 below with $T = R^2 = r^2$ and $\alpha = (4/3)\sigma = 2\gamma = 4\beta = 8\eta = 4$. The gap (of order r^2) between the two inner-cylinders is necessary, dictated by the parabolic nature of the equation.

As in the elliptic case, the parabolic Harnack inequality (8) implies the Hölder continuity of the corresponding local solution (this continuity was first obtained by Nash in [46]).

Fig. 1. The cylinders $Q_-, Q_+ \subset Q$

For a positive solution in Q,

$$\sup_{Q_-}\{u\} \le H_0 \inf_{Q_+}\{u\}.$$

Again, in the context of weighted Riemannian manifolds, we may consider (8) as a property, call it (PHI), that may or may not be satisfied. For complete Riemannian manifolds (M, g) of dimension n with non-negative Ricci curvature, P. Li and S.T. Yau proved that any positive solution u of the heat equation in $(s, s, +r^2) \times B$, $B = B(x, r)$, satisfies

$$|\nabla \log u|^2 - 2\partial_t \log u \le C(n)\left(\frac{1}{r^2} + \frac{1}{t}\right) \text{ in } (0, r^2) \times B(x, r/2).$$

For global positive solution u of the heat equation, they obtain the refined optimal inequality

$$|\nabla \log u|^2 - \partial_t \log u \le \frac{n}{2t} \text{ in } (0, \infty) \times M.$$

The first of these gradient estimates implies that (8) holds on manifolds with non-negative Ricci curvature. The second gradient inequality yields, for any $\epsilon \in (0, 1)$, the very precise two-sided heat kernel bound

$$(9) \qquad \frac{c(\epsilon)}{V(x, \sqrt{t})} e^{-\frac{d(x,y)^2}{4(1+\epsilon)t}} \le p(t, x, y) \le \frac{C(\epsilon)}{V(x, \sqrt{t})} e^{-\frac{d(x,y)^2}{4(1-\epsilon)t}},$$

as well as the companion gradient estimate

$$(10) \qquad |\nabla_y p(t, x, y)| \le \frac{C(\epsilon)}{\sqrt{t} V(x, \sqrt{t})} e^{-\frac{d(x,y)^2}{4(1-\epsilon)t}}$$

See [43].

3.2. The characterization of (PHI)

In contrast to the fact that we do not have a precise description of those complete weighted Riemannian manifolds that satisfy the elliptic

Harnack inequality, there is a very good description of the class of complete weighted Riemannian manifolds satisfying the parabolic version (PHI). This theorem also applies to weighted manifolds with boundary as long as the Neumann condition is assumed.

Theorem 3.1 ([26, 49]). *Let (M, g) be a weighted complete Riemannian manifold. The following three properties are equivalent:*

- *The parabolic Harnack inequality* (PHI).
- *The two-sided heat kernel bound* $((t, x, y) \in (0, \infty) \times M \times M)$

$$(11) \qquad \frac{c_1}{V(x, \sqrt{t})} e^{-C_1 \frac{d(x,y)^2}{t}} \le p(t, x, y) \le \frac{C_2}{V(x, \sqrt{t})} e^{-c_2 \frac{d(x,y)^2}{t}}.$$

- *The conjunction of*
  - *The volume doubling property*

  $$\forall\, x \in M, \ r > 0, \ \ V(x, 2r) \le DV(x, r).$$

  - *The Poincaré inequality ($\forall\, x \in M, \ r > 0, \ B = B(x, r)$)*

  $$\forall\, f \in \mathrm{Lip}(B), \ \ \int_B |f - f_B|^2 d\mu \le Pr^2 \int_B |\nabla f|^2 d\mu,$$

  where f_B is the mean of f over B.

Here $\mathrm{Lip}(B)$ denotes the space of bounded Lipschitz functions in B. This space can be replaced by the space of smooth functions in B that are bounded with bounded gradient, or by the natural Sobolev space $W^1(B)$ of those functions in $L^2(B)$ whose first derivatives in the sense of distributions can be represented by functions in $L^2(B)$. Assuming the doubling property, the Poincaré inequality can be replaced by

$$\forall\, f \in \mathcal{C}_c^\infty(M), \ \ \int_B |f - f_B|^2 d\mu \le Pr^2 \int_{kB} |\nabla f|^2 d\mu,$$

where $B = B(x, r)$, $kB = B(x, kr)$, $x \in M$, $r > 0$ and f_B is the mean of f over B. It is in this weaker form that the Poincaré inequality is often obtained. See [26, 49, 50] and also [51, Chapter 5].

The doubling property implies that for all $x, y \in M$ and $0 < r < R < \infty$

$$\frac{V(y, R)}{V(x, s)} \le D_1 \left(\frac{d(x, y) + R}{r} \right)^\alpha$$

and, if M is assumed to be non-compact,

$$\frac{V(x, R)}{V(x, r)} \ge d_1 \left(\frac{R}{r} \right)^\beta,$$

for some $0 < \beta \leq \alpha < \infty$.

Another interesting characterization of the class of manifold that satisfy (PHI) is as follows: A complete weighted manifold M satisfies (PHI) if and only if the Riemannian product $\mathbb{R} \times M$ satisfies the elliptic Harnack inequality. See [38] for details and further results.

3.3. Examples of weighted manifolds satisfying (PHI)

Here is a list of examples with additional comments in each case.

- Complete Riemannian manifolds with non-negative Ricci curvature. In this case, the doubling property follows from the celebrated Bishop-Gromov volume comparison. The Poincaré inequality follows from the work [11] of P. Buser. See also [51, Sect. 5.6.3]. The parabolic Harnack inequality and the two-sided heat kernel bound were first obtained by Li and Yau in [43].
- Convex domains in Euclidean space. The doubling property and Poincaré inequality are well-known results in this case. The Harnack inequality and heat kernel bound can be derived by the Li-Yau argument, at least for smooth convex domains (convexity of the boundary is similar to non-negative Ricci curvature). Of course, the Neumann boundary condition is assumed.
- Complements of any convex domain. It is amusing and instructive that both convex domains and their complements satisfy (PHI). In the case of the complement of a convex domain, note that the distance is the intrinsic geodesic distance of the domain (for convex domains, the intrinsic geodesic distance equals the Euclidean distance). That (PHI) holds in this case is a recent result of the author and his graduate student P. Gyrya. More generally, (PHI) holds in inner uniform domains (complements of convex domains are inner uniform but unbounded convex domains are not).
- Connected Lie groups with polynomial volume growth. These are connected Lie groups such that for any compact neighborhood K of the origin, $\forall n$, $|K^n| \leq Cn^A$ for some constants C, A. Here $K^n = \{k = k_1 \dots k_n : k_i \in K\}$ and $|K^n|$ is the Haar measure of K^n. Nilpotent Lie groups are always of this type. By an important result of Guivarc'h, there must then exist an integer D such that $\forall n$, $c_1 n^D \leq |K^n| \leq C_1 n^D$. This implies the doubling property for any left-invariant Riemannian metric. Concerning the Poincaré inequality, see, e.g., [51].

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For the parabolic Harnack inequality, see [63]. It is interesting to note that doubling, Poincaré and (PHI) also hold for the sub-Laplacians of the form $\Delta = \sum_1^k X_i^2$ associated with a family of left invariant vector fields $\mathcal{F} = \{X_i, 1 \leq i \leq k\}$, as long as $\mathcal{F}$ generates the Lie algebra (this is called Hörmander condition). See [63].

- Let (M, g) be a Riemannian manifold which covers a compact manifold with deck transformation group Γ. The group Γ is finitely generated and, choosing a finite symmetric generating set, we can consider its volume growth. If Γ has polynomial volume growth then (M, g) satisfies (PHI). See, e.g., [20, 50, 52].

- Assume that M, N are two complete Riemannian manifolds and G is a group of isometries of M such that $M/G = N$. Then, if M satisfies (PHI) so does N. See,e.g., [49, 50].

- Consider the Euclidean space $\mathbb{R}^n$, $n \geq 2$, with weight $(1 + |x|^2)^{\alpha/2}$, $\alpha \in (-\infty, \infty)$. This is a complete weighted manifold. It satisfies (PHI) if and only if $\alpha > -n$. It satisfies the elliptic Harnack inequality for all α. See [33] for this and other examples in this spirit.

- Any weighted complete Riemannian manifold with bounded geometry (see Section 2.4) which is (volume) quasi-isometric to a complete weighted manifold satisfying (PHI) also satisfies (PHI). See [41, 20].

3.4.   Some consequences

In this subsection, I describe two consequences of the parabolic Harnack inequality (PHI) that will play a role in Lecture III. They concern the Dirichlet heat kernel in the complement of a compact set and the hitting probability of a compact set. The main references for these results are [31, 32].

3.4.1. *The Dirichlet heat kernel in $\Omega = M \setminus K$* Let K be a compact set with non-empty interior in a complete weighted manifold M and set $\Omega = M \setminus K$. We are concerned with the fundamental solution $p_\Omega(t, x, y)$ of the heat equation in Ω with Dirichlet boundary condition along $\partial\Omega$ (the reader can assume that K as smooth boundary but it is irrelevent for our purpose). Note that we always have $p_\Omega(t, x, y) \leq p(t, x, y)$.

Theorem 3.2 ([31]). *Assume that M satsifies* (PHI) *and is transient, that is, $\int_1^\infty \frac{ds}{V(x, \sqrt{s})} < \infty$. Then there exist $\delta, c, C \in (0, \infty)$ such that for all $(t, x, y) \in (0, \infty) \times (M \setminus K_\delta)^2$,*

$$cp(Ct, x, y) \leq p_\Omega(t, x, y) \leq p(t, x, y).$$

Here, K_δ is the δ-neighborhood of K. This theorem says that, when M is transient and satisfies (PHI), the Dirichlet heat kernel in Ω is comparable to the heat kernel of M away from $\partial\Omega$. The hypothesis that M is transient is essential. Note that the theorem implies that Ω must be connected at infinity.

To state a result concerning the case when M is recurrent, that is, when $\int_1^\infty \frac{ds}{V(x,\sqrt{s})} = \infty$, we need an additional assumption.

Definition 3.3. *We say that M satisfies* (RCA) *(this stands for relatively connected annuli) if there is a point o and a constant A such that for any $r > A^2$ and any two points $x, y \in M$ with $d(o, x) = d(o, y) = r$ there is a continuous path in $B(o, Ar) \setminus B(o, r/A)$ connecting x to y.*

Theorem 3.4 ([31]). *Assume that M satsifies* (PHI), (RCA) *and is recurrent. Then there exist $\delta, c_i \in (0, \infty)$, $i = 1, \ldots, 4$ such that for all $(t, x, y) \in (0, \infty) \times (M \setminus K_\delta)^2$,*

$$c_1 D(t, x, y) p(c_2 t, x, y) \leq p_\Omega(t, x, y) \leq c_3 D(t, x, y) p(c_4 t, x, y)$$

where

$$D(t, x, y) = \frac{H(|x|)H(|y|)}{(H(|x|) + H(\sqrt{t}))(H(|y|) + H(\sqrt{t}))}$$

with $|x| = \sup\{d(x, k) : k \in K\}$ and

$$H(r) = 1 + \int_0^r \frac{s e^{-1/s}}{V(o, s)} ds, \ \ o \in K \text{ fixed.}$$

For instance if $M = \mathbb{R}^2$ then $H(r) \simeq \log(2 + |x|)$.

3.4.2. *Hitting probabilities* Let X_t be the strong Markov process associated with our heat semigroup (i.e., Brownian motion on M). In this section we consider the hitting probability

$$\psi_K = \mathbb{P}_x(\exists s \in [0, t] : X_s \in K).$$

This is a solution of the heat equation in $\Omega = M \setminus K$ taking the boundary value 1 on $\partial\Omega$. It is a very important solution from many different viewpoints. We assume that K is a compact set with non-empty interior and o in an interior point of K. The notation is as in the previous section.

Theorem 3.5 ([32]). *Assume that M satisfies* (PHI) *and is transient, that is, $\int_1^\infty \frac{ds}{V(x,\sqrt{s})} < \infty$. Then, for any $\delta > 0$ there exist $c, C \in (0, \infty)$ such that for all $(t, x) \in (0, \infty) \times (M \setminus K_\delta)$ we have*

$$\frac{c|x|^2}{V(o, |x|)} e^{-C|x|^2/t} \leq \psi_K(t, x) \leq \frac{C|x|^2}{V(o, |x|)} e^{-c|x|^2/t} \text{ if } t < 2|x|^2$$

and

$$c \int_{|x|^2}^{t} \frac{1}{V(o, \sqrt{s})} ds \leq \psi_K(t, x) \leq C \int_{|x|^2}^{t} \frac{1}{V(o, \sqrt{s})} ds \ \ if \ t \geq 2|x|^2.$$

Moreover, for all large enough δ and $(t, x) \in (\delta^2, \infty) \times (M \setminus K_\delta)$,

$$\frac{c}{V(o, \sqrt{t})} e^{-C|x|^2/t} \leq \psi'_K(t, x) \leq \frac{C}{V(o, \sqrt{t})} e^{-c|x|^2/t}.$$

The hitting probability estimates in the recurrent case are very interesting but we refer the reader to [32, Sec. 4.4].

§4. Lecture III: The heat kernel on manifold with ends

The aim of this Lecture is to describe the results of [30, 34] which provide two-sided estimates that are fundamentally different from (11). This is joint work with A. Grigor'yan. We investigate the heat kernel on complete weighted manifolds of the form

$$M = M_1 \# \ldots \# M_k,$$

that is, manifold that are the connected sum of a finite number k of manifolds M_i, $1 \leq i \leq k$. More precisely, this means that M is the disjoint union $M = K \cup E_1 \cup \cdots \cup E_k$ where K is a compact with smooth boundary – we refer to it as *the cenral part* – and each E_i is isometric to the complement of a compact set K_i with smooth boundary in M_i. If M is weighted then we assume that the M_i's are weighted. The weight on M and the weight on M_i coincide on E_i (with the obvious identification). Technically, it is actually very convenient to allows the M_i to have a boundary since we can then consider the case when $M_i = \overline{E_i}$. In addition, the simplest examples are actually examples of domains in $\mathbb{R}^n$ (e.g., with $n = 3$) in which case we assume the Neumann condition along the boundary. In this context, for any $x \in M$, we let $i_x = i$ if $x \in E_i$, $i_x = 0$ if $x \in K$ (the choice of what i_x means when $x \in K$ will never play an important role).

Our goal is to study the heat kernel on $M = M_1 \# \ldots \# M_k$ when each M_i satisfies (PHI), i.e., satisfies the two-sided heat kernel bound (11). This is done by using a gluing technique developed in [34]. The idea is to reduce the problem as much as possible to estimates that depend on each end separately. Since each end satisfies (PHI), we know a lot about the heat equation on each end. The estimates of the Dirichlet heat kernel on E_i and of the hitting probability of K starting from $x \in E_i$ play a crucial role in this technique. In addition, and this is the only

input that depends globally on M, we need an estimate of the heat kernel $p(t, x, y)$ when x, y are in the central part K. It turns out that the structure of the heat kernel bound depends in a crucial ways on whether or not the manifold M is transient and also, if M is transient, on whether or not every end is transient.

4.1.   The case when every end is transient

In this section we assume that $M = M_1 \# \ldots \# M_k$ with every M_i being a transient manifold satisfying (PHI). Because M_i satisfies (PHI), transience means $\int_1^\infty \frac{ds}{V_i(o, \sqrt{s})} < \infty$. Here and in what follows o is a fixed point in the interior of the compact K and

$$V_i(x, r) = \mu(B(x, r) \cap (K \cup E_i)), \quad x \in K \cup E_i$$

is the E_i-restricted volume growth function. We set

$$V_0(r) = \min_i \{V_i(o, r)\}.$$

Note that the end E_i that yields the smallest volume $V_i(o, r)$ may depend on r. For $x \in M$, set

$$|x| = \sup_{k \in K} d(k, x)$$

and

$$i_x = i \text{ if } x \in E_i \text{ with the convention that } K = E_0.$$

Define $H(x, t)$ on $M \times (0, \infty)$ by the formula

$$(12) \qquad H(x, t) = \min \left\{ 1, \frac{|x|^2}{V_{i_x}(o, |x|)} + \left(\int_{|x|^2}^t \frac{ds}{V_{i_x}(o, \sqrt{s})} \right)_+ \right\}.$$

Note that $H(x, t) \simeq 1$ if $|x|$ stays bounded and $H(x, t)$ is comparable to the hitting probability $\psi_K(t, x)$ if $x \in E_i$ and away from K (this probability can be computed in M_i!). See Section 3.4.2.

Let $d_\emptyset(x, y)$ be the infimum of the length of rectifiable curves joining x to y without entering K. Let $d_+(x, y)$ be the infimum of the length of rectifiable curves joining x to y and intersecting K. Note taht if x, y are in the same end and away from K then $d_\emptyset(x, y) = d(x, y)$ whereas, if x, y are in different ends, then $d_+(x, y) = d(x, y)$.

Theorem 4.1 ([34]). *Assume that $M = M_1 \# \ldots \# M_k$ is the comnnected sum of the complete non-compact weighted Riemannian manifolds M_i, $1 \le i \le k$, where each M_i is transient and satisfies* (PHI). *Then the*

*heal kernel $p(t, x, y)$ on M is bounded above and below by expressions of
the type*

$$\frac{c_1}{\sqrt{V_{i_x}(x, \sqrt{t})V_{i_y}(y, \sqrt{t})}} \exp\left(-c_2 \frac{d_\emptyset(x,y)^2}{t}\right) +$$

$$c_3 \left(\frac{H(x,t)H(y,t)}{V_0(\sqrt{t})} + \frac{H(x,t)}{V_{i_y}(o, \sqrt{t})} + \frac{H(y,t)}{V_{i_x}(o, \sqrt{t})}\right) \exp\left(-c_4 \frac{d_+(x,y)^2}{t}\right).$$

To illustrate this result in a simple case, set $M_i = \mathbb{R}^N/\mathbb{Z}^{N-N_i}$ for
some $N_1, \ldots, N_k$, with $n = \min\{N_i\} > 2$ and $N \geq \max\{N_i\}$. In this
case, the end M_i has volume growth $V_i(r) \simeq r^{N_i}$ for large r. For sim-
plicity, assume that $x \in E_i$, $y \in E_j$ with $i \neq j$ and that $|x|, |y| \leq \sqrt{t}$.
Then the theorem above yields the two-sided bound

$$p(t, x, y) \simeq \frac{1}{t^{n/2}|x|^{N_i-2}|y|^{N_j-2}} + \frac{1}{t^{N_i/2}|y|^{N_j-2}} + \frac{1}{t^{N_j/2}|y|^{N_i-2}}.$$

4.2. The case when M is transient

The case when M is transient but at least one end M_i is not is rather
interesting. It is completely different from, but can be reduced to, the
case when every end is transient. The reduction is via the technique of
Doob transfoms. More precisely, we assume that $M = M_1 \# \ldots \# M_k$ is
transient with each M_i satisfying (PHI). We assume further that each
M_i satisfies (RCA) (see Defnition 3.3). Then there exists a positive
harmonic function h on M such that (see [31, 58])

$$h(x) \simeq 1 + \left(\int_1^{|x|^2} \frac{ds}{V_{i_x}(o, \sqrt{s})}\right)_+.$$

Theorem 4.2 ([33, 34])**.** *The ends $\widetilde{M}_i$ of the weighted manifold*

$$\widetilde{M} = (M, h^2 d\mu) = \widetilde{M}_1 \# \ldots \# \widetilde{M}_k$$

are transient and satisfy (PHI)*.*

The classical Doob transform technique shows that the heat kernel
on M and the heat kernel on $\widetilde{M}$ are related by a simple formula. This
and Theorem 4.1 yields the following result.

Theorem 4.3. *Consider $M = M_1 \# \cdots \# M_k$. Assume that M is
transient. Assume that each M_i satisfies* (PHI) *and* (RCA)*. Then the*

heat kernel is bounded above and below by expressions of the type

$$h(x)h(y) \times \left(\frac{1}{\sqrt{\widetilde{V}_{i_x}(x, \sqrt{t})\widetilde{V}_{i_y}(y, \sqrt{t})}} \exp\left(-\frac{d_\emptyset^2(x,y)}{t}\right) + \right.$$

$$\left. \left(\frac{\widetilde{H}(x,t)\widetilde{H}(y,t)}{\widetilde{V}_0(\sqrt{t})} + \frac{\widetilde{H}(x,t)}{\widetilde{V_{i_y}}(o, \sqrt{t})} + \frac{\widetilde{H}(y,t)}{\widetilde{V_{i_x}}(o, \sqrt{t})} \right) \exp\left(-\frac{d_+^2(x,y)}{t}\right) \right).$$

Here $\widetilde{}$ means that the corresponding object is computed on the weighted manifold $\widetilde{M} = (M, h^2 d\mu)$.

Let us point out that this theorem covers a great variety of different cases. For each (t, x, y) one (or more) of the terms in the theorem will dominate the other terms. It is not always obvious to guess which term will dominate. Under the general hypotheses of the theorem, it is not always possible to rank the ends from smallest to largest. Indeed, which end is smallest (or largest), viewed from the central part K, may well depend on the scale r at which one look at them. One end may be the smallest for a long while but later turn out to be the largest end, assymptotically as r tends to infinity. Since the stated estimates are uniform in t, x, y, they do capture such phenomenon.

Corollary 4.4 ([34]). *Assume that $M = M_1 \# \cdots \# M_k$ is transient with each M_k satisfying* (PHI) *and* (RCA). *Then*

- $\sup_{x,y}\{p(t,x,y)\} \simeq \max_i\{V_i(o, \sqrt{t})^{-1}\}$
- $\sup_y\{p(t,x,y)\} \simeq \max_i\{[\eta_i(\sqrt{t})V_i(o, \sqrt{t})]^{-1}\}$
- $p(t,x,y) \simeq \max_i\{[\eta_i(\sqrt{t})^2 V_i(o, \sqrt{t})]^{-1}\}$

with

$$\eta_i(r) := 1 + \left(\int_1^{r^2} \frac{ds}{V_i(o, \sqrt{s})} \right)_+.$$

4.3. An explicit example

We now describe the application of the theorem of the previous section in the case of a very explicit example depicted in Figure 2. This example is taken from [34].

For the domain of Figure 2 (with Neumann boundary condition), we ask the following questions:

- What is the large time behavior of the heat kernel $p(t, x, y)$ for fixed x, y?
- What is the behavior of $\phi(t, x) = \sup_y\{p(t,x,y)\}$ for a fixed x?
- What is the behavior of $\phi(t) = \sup_{x,y}\{p(t,x,y)\}$?

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Fig. 2. A 3-d transient Euclidean domain with 3 ends
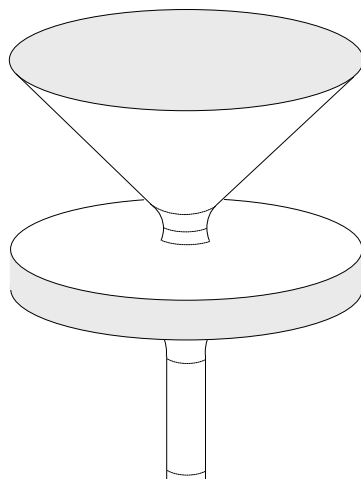
- What is the rough location and shape of

$$\mathrm{HOT}_\epsilon(t,x) = \{y \in M : p(t,x,y) \geq \epsilon\phi(t,x)\}?$$

The bound of Theorem 4.3 allows us to answer all these questions.

- For any fixed x, y, $p(t,x,y) \simeq 1/(t(\log t)^2)$ as t tends to infinity.
- For any fixed x, $\phi(t,x) \simeq 1/t$ as t tends to infinity.
- $\phi(t) \simeq 1/\sqrt{t}$ as t tends to infinity.
- For $\epsilon > 0$ small enough , any fixed x, and t large enough, the hot-point region $\mathrm{HOT}_\epsilon(t,x)$ is situated in the small cylindric end at the bottom of Figure 2 at a distance of order $\sqrt{t}$ form the central part K of M and has width of order $\sqrt{t}$. See Figure 3 which shows various temperature regions in a schematic rendering of the domain of Figure 2.

In Figure 3, $\mathcal{R}^1$ represents the cylindric bottom part (volume growth r^1), $\mathcal{R}^2$ represents the planar middle part (volume growth r^2), and $\mathcal{R}^3$ represents the conical top part (volume growth r^3). The function $\mathcal{H}(y)$ is defined by $\mathcal{H}(y) = p(t,x,y)/\phi(t,x)$ where we think of x as fixed and of t as fixed but very large.

Fig. 3. Temperatures in the Euclidean domain of Figure 2
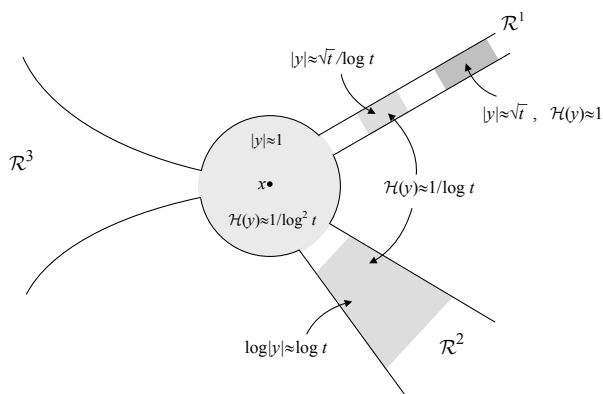
4.4. Brief outline of the proof of Theorem 4.1

The proof of Theorem 4.1 depends on a number of results and estimates of independent interest, in particular, those describe above in Sections 3.4.1-3.4.2. The idea is to reduce things as much as possible to estimates that depends on each end taken separately. Then, one needs to "glue" these various estimate together. This is achieved via a gluing technique developed in [34]. A rough account of this technique is given by the very general bound described below.

Let Ω_1 and Ω_2 be two open sets in M with boundaries Γ_1 and Γ_2 respectively. Assume that Γ_2 separates Ω_2 from Γ_1 in the sense that either Ω_1, Ω_2 are disjoint or $\Omega_2 \subset \Omega_1$.

Let $\psi_i = \psi_{\Gamma_i}$ be the hitting probability defined in Section 3.4.2 and p_{Ω_1} be the Dirichlet heat kernel in Ω_1 as in Section 3.4.1. Set

$$\overline{G}(t) := \int_0^t \sup_{v \in \Gamma_1, w \in \Gamma_2} p(s,v,w)ds, \quad \underline{G}(t) := \int_0^t \inf_{v \in \Gamma_1, w \in \Gamma_2} p(s,v,w)ds.$$

Then, for all $x \in \Omega_1$, $y \in \Omega_2$, and $t > 0$,

$$
\begin{aligned}
p(t, x, y) \;\leq\;\; & p_{\Omega_1}(t, x, y) \\
+\;\; & 2 \left(\sup_{s \in [t/4, t]} \sup_{v \in \Gamma_1, w \in \Gamma_2} p(s, v, w) \right) \psi_1(t, x) \psi_2(t, y) \\
+\;\; & \overline{G}(t) \left[\sup_{s \in [t/4, t]} \psi_1'(s, x) \right] \psi_2(t, y) \\
+\;\; & \overline{G}(t) \left[\sup_{s \in [t/4, t]} \psi_2'(s, y) \right] \psi_1(t, x)
\end{aligned}
$$

and

$$
\begin{aligned}
p(t, x, y) \;\geq\;\; & (1/2) p_{\Omega_1}(t, x, y) \\
+\;\; & \left[\inf_{s \in [t/4, t]} \inf_{v \in \Gamma_1, w \in \Gamma_2} p(s, v, w) \right] \psi_1(\tfrac{t}{4}, x) \psi_2(\tfrac{t}{4}, y) \\
+\;\; & \underline{G}(\tfrac{t}{4}) \left[\inf_{s \in [t/4, t]} \psi_1'(s, x) \right] \psi_2(\tfrac{t}{4}, y) \\
+\;\; & \underline{G}(\tfrac{t}{4}) \left[\inf_{s \in [t/4, t]} \psi_2'(s, y) \right] \psi_1(\tfrac{t}{4}, x).
\end{aligned}
$$

The reader should compare the structure of these bounds to the bound stated in Theorem 4.1. See [34] for further details.

§5.   Lecture IV: Heat kernels in inner uniform domains

In this last lecture, I describe joint work with Pavel Gyrya concerning the Neumann and Dirichlet heat kernel in Euclidean domain. The goal of this work is to obtain sharp heat kernel bounds for the heat kernel with Dirichlet boundary condition in certain domains. The simplest case of a domain of interest is the upper half space $U = \mathbb{R}_+^n = \{x : x_n > 0\}$.

The Neumann heat kernel in $U = \mathbb{R}_+^n = \{x : x_n > 0\}$ equals

$$
p_U^N(t, x, y) = \frac{1}{(4\pi t)^{n/2}} \left(e^{-\frac{\|y - x\|^2}{4t}} + e^{-\frac{\|y' - x\|^2}{4t}} \right).
$$

The Dirichlet heat kernel in $U = \mathbb{R}_+^n = \{x : x_n > 0\}$ equals

$$
p_U^D(t, x, y) = \frac{1}{(4\pi t)^{n/2}} \left(e^{-\frac{\|y - x\|^2}{4t}} - e^{-\frac{\|y' - x\|^2}{4t}} \right)
$$

Here, y' is the symmetric of y w.r.t. hyperplane $\{x_n = 0\}$.

For the Neumann heat kernel, it is plain that

$$p_U^N(t, x, y) \simeq t^{-n/2} e^{-\frac{\|y-x\|^2}{t}}.$$

For the Dirichlet heat kernel, it is not immediate to see that, in fact,

$$p_U^D(t, x, y) \simeq \frac{x_n y_n}{t^{n/2}(x_n + \sqrt{t})(y_n + \sqrt{t})} e^{-\frac{\|y-x\|^2}{4t}}.$$

A natural and important problem is to obtain such results for more general domains.

For instance, given a (finite or) countable family $\mathbf{f} = \{(x_i, y_i))\} \subset \mathbb{R}_+^2$ of points in the upper-half plane, let $\mathbb{R}_{+\mathbf{f}}^2$ be the upper-half plane with the vertical segments $s_i = \{z = (x_i, y) : 0 < y \leq y_i\}$ deleted. When can one obtain good heat kernel estimates (with either Neumann or Dirichlet boundary condition) in $\mathbb{R}_{+\mathbf{f}}^2$?

Fig. 4. A slit upper-half plane

(x_i, y_i)

x_i
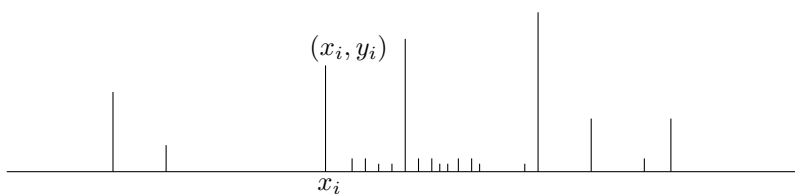
5.1. Uniform and inner uniform domains

Recall the following definitions illustrated in Figure 6.

Definition 5.1. *A domain U is uniform if there are constants $c_0, C_0 \in (0, \infty)$ such that for any two points x,y in U there exists a curve joining x to y of length at most $C_0 d(x, y)$ and such that, for any z on the curve,*

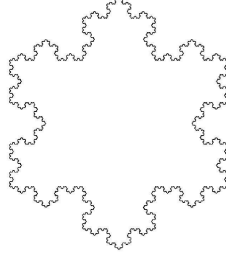$$\operatorname{dist}(z, U^c) \geq c_0 \frac{d(x, z)d(y, z)}{d(x, y)}.$$

Good examples of uniform domains are:

- Domain above the graph of a Lipschitz function Φ:

$$U = \{x = (x_1, \ldots, x_n) : \Phi(x_1, \ldots, x_{n-1}) < x_n\}.$$

- The inside and outside of the snow flake

Fig. 5. Approximation of a snow flake

Let $d_U(x,y)$ be the inner distance in U between x and y. By definition, $d_U(x,y)$ is obtained by minimizing the length of curves joining x to y in U.

Definition 5.2. *A domain U is inner uniform if there are constants $c_0, C_0 \in (0, \infty)$ suh that for any two points x,y in U there exists a curve joining x to y of length at most $C_0 d_U(x,y)$ and such that, for any z on the curve,*

$$\operatorname{dist}(z, U^c) \geq c_0 \frac{d_U(x,z) d_U(y,z)}{d_U(x,y)}.$$

Good examples of inner uniform domains are:

- The slit half-plane $\mathbb{R}^2_{+\mathbf{f}}$ is inner uniform if and only if there is a constant $c > 0$ such that for any pair (i,j), $|x_i - x_j| \geq c \min\{y_i, y_j\}$. Such domains are never uniform if there is at least one non trivial slit.
- The complement C^c of any convex set C in $\mathbb{R}^n$ (such complement will often not be uniform), e.g., the outside of a parabola in the plane. Note that the inside of the parabola is neither uniform nor inner uniform.

Definition 5.3. *Let $(\widetilde{U}, d_U)$ be the abstract completion of (U, d_U).*

5.2. The Neumann heat kernel in an inner uniform domain

Given a Domain $U \subset \mathbb{R}^n$, let $W^1(U)$ be the subspace of $L^2(U)$ of those functions f whose first order partial dervatives in the sense of distributions can be represented by locally integrable functions that belong to $L^2(U)$.

Fig. 6. The inner uniform condition
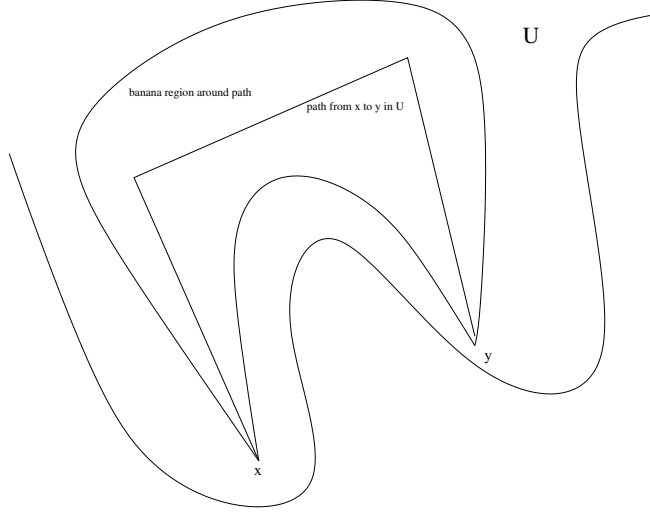
Theorem 5.4 ([36, 37])**.** *Let U be an inner uniform domain. Then the heat kernel $p_U^N(t,x,y)$ associated with the Dirichlet form*

$$\mathcal{E}_U^N(f,f) = \int_U |\nabla f|^2 d\lambda, \ \ f \in W^1(U),$$

is a continuous function of $(t,x,y) \in (0,\infty) \times U \times U$ which satisfies

$$c_1 t^{-n/2} e^{-\frac{d_U(x,y)^2}{c_2 t}} \leq p_U^N(t,x,y) \leq c_3 t^{-n/2} e^{-\frac{d_U(x,y)^2}{c_4 t}}.$$

This is proved by showing that the Dirichlet form $(\mathcal{E}_U^N, W^1(U))$ is regular on $\widetilde{U}$ and satisfies the doubling property and a Poincaré inequality (see Section below).

5.3. The Dirichlet heat kernel in an unbounded inner uniform domain

Given a domain U, we consider the subspace $W_0^1(U)$ of $W^1(U)$ which is the closure of $\mathcal{C}_c^\infty(U)$ in $W^1(U)$ for the norm $(\|f\|_2^2 + \|\nabla f\|_2^2)^{1/2}$. This defines a regular Dirichlet form $\mathcal{E}_U^D(f,f) = \int_U |\nabla f|^2 d\lambda, \ f \in W_0^1(U)$. The associate heat kernel, $p_U^D(t,x,y)$ is always bounded by

$$p_U^D(t,x,y) \leq (4\pi t)^{-n/2} e^{-\frac{\|x-y\|^2}{4t}}$$

but this is a crude estimate.

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Definition 5.5. *Given a domain U, we call* harmonic profile *of U any function $h \in \mathcal{C}^\infty(U)$ such that: (a) $\Delta h = 0$, (b) $h > 0$ in U, (c) $h \in W^1_{0,\mathrm{loc}}(U)$.*

Such functions do not exist if U is bounded. The set of harmonic profiles form a positive cone and, in general, this cone might contains more than one half-line.

The following result follows from the boundary Harnack principle obtained in [1, 2]. See [36, 37] for details.

Theorem 5.6 ([1, 2, 36, 37]). *Let U be an unbounded inner uniform domain. Then U admits a harmonic profile h and any other harmonic profile h' satisfies $h' = ah$ for some $a > 0$. Moreover, the function h has the following properties:*

- *For any $\epsilon \in (0, 1)$, there exists a constant $C = C_\epsilon$ such that $\forall\, x \in U$, $r > 0$, $y, z \in U$ with $d_U(x, y) < r$, $d_U(x, z) < r$ and $d(z, U^c) > \epsilon r$, we have $h(y) \le Ch(z)$.*
- *The measure $h^2 d\lambda$ on (U, d_U) has the doubling property.*

This is the key to the follwoing precise heat kernel estimate.

Theorem 5.7 ([36, 37]). *Let U be an unbounded inner uniform domain. Let h be a harmonic profile for U. Let $V_{h^2}(x, r) = \int_{\{d_U(x,y)<r\}} h^2 d\lambda$. The Dirichlet heat kernel in U, $p^D_U(t, x, y)$, is bounded by*

$$\frac{c_1 h(x)h(y)}{\sqrt{V_{h^2}(x, \sqrt{t})V_{h^2}(y, \sqrt{t})}} e^{-\frac{d_U(x,y)^2}{c_2 t}} \le p^D_U(t, x, y)$$

and
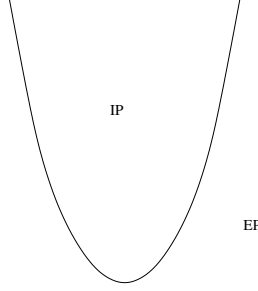
$$p^D_U(t, x, y) \le \frac{c_3 h(x)h(y)}{\sqrt{V_{h^2}(x, \sqrt{t})V_{h^2}(y, \sqrt{t})}} e^{-\frac{d_U(x,y)^2}{c_4 t}}.$$

As an explicit interesting example depicted in Figure 7, consider the exterior of the parabola in the plane, that is, the domain $U = \mathrm{EP} = \{x = (x_1, x_2) = x_2 < x_1^2\}$. Then

$$h(x) = \sqrt{2\left(\sqrt{x_1^2 + (1/4 - x_2)^2} + 1/4 - x_2\right) - 1}.$$

In particular, for any fixed $x, y \in U$, $P^D_U(t, x, y) \simeq t^{-3/2}$ as t tends to infinity.

Fig. 7. The domain outside the parabola

5.4.   Inner uniform domains and Harnack-type Dirichlet spaces

One of the key to the heat kernel estimates described in the previous two sections is the extension of Theorem 3.1 to the abstract setting of regular strictly local Dirichlet spaces. This extension was obtained by K. Th. Sturm in a series of papers [54, 55, 56]. See also the related work of Biroli and Mosco [10].

Without entering into the details, a Harnack-type Dirichlet space is a regular strictly local Dirichlet space $(M, \lambda, \mathcal{E}, \mathcal{F})$ with the following additional properties:

- (a) M is a locally compact connected metrizable space equiped with a positive Radon measure λ and $(\mathcal{E}, \mathcal{F})$ is a regular strictly local Dirichlet form on $L^2(U, \lambda)$.
- (b) The intrinsic distance d (associated to $(\mathcal{E}, \mathcal{F})$) defines the topology of M and (M, d) is a complete metric space.
- (c) The space (M, d, λ) has the doubling property and satisfies the Poincaré inequality

$$\forall\, B = B(x, r), \ \ \forall\, f \in \mathcal{F}, \ \ \int_B |f - f_B|^2 d\lambda \le Pr^2 \int_B d\Gamma(f, f).$$

In this Poincaré inequality, $B(x, r)$ is the intrinic metric ball of radius r around x and $d\Gamma$ is the energy measure of $\mathcal{E}$ (in the classical case, $d\Gamma(f, f) = |\nabla f|^2 d\lambda$). For any locally integrable function f, f_B is the mean of f over B.

On any Harnack-type Dirichlet space, the associated heat semigroup admits a continuous kernel $p(t, x, y)$ satisfying

$$\frac{c_1}{V(x, \sqrt{t})} e^{-\frac{d(x,y)^2}{c_2 t}} \le p(t, x, y) \le \frac{c_3}{V(x, \sqrt{t})} e^{-\frac{d(x,y)^2}{c_4 t}}.$$

See [55, 56] and [36, 37, 38].

The theorems stated in the previous two sections and concerning the Neumann heat kernel p_U^N and the Dirichlet heat kernel p_U^D on an unbounded inner uniform domain U in $\mathbb{R}^n$ are obtained by applying the theory of Harnack-type Dirichlet spaces to certain Dirichlet forms on the abstract completion $\widetilde{U}$ of (U, d_U). Note that this abstract completion is not, in general, a subset of $\mathbb{R}^n$. For instance the result concerning the Neumann heat kernel p_U^N on an inner uniform domain (Theorem 5.4) is obtained by showing that the Dirichlet space $(\widetilde{U}, \lambda, \mathcal{E}_U^N, W^1(U))$ is of Harnack type. The treatment of the Dirichlet heat kernel P_U^D is more intricate as it involves the use of a h-transform where h is the harmonic profile of the domain. However, the main point is again to show that a certain Dirichlet space on $\widetilde{U}$ is of Harnack type.

A far reaching generalization of Theorems 5.4-5.7 is that similar results hold for unbounded inner uniform domains in Harnack-type Dirichlet spaces that admits a carré du champ. See [36, 37] for details.

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