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HEAT KERNELS ON NON-COMPACT RIEMANNIAN MANIFOLDS: A PARTIAL SURVEY

Thierry COULHON

Pour Hubert

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1. Introduction

Let M be a complete, non-compact Riemannian manifold, Δ the Laplace-Beltrami operator on M , $e^{t\Delta}$, $t > 0$, the heat semi-group, and $p_t(x, y)$, $x, y \in M$, $t > 0$, the heat kernel.

The main question we shall address in this survey is: how can one connect the behaviour of $\sup_{x \in M} p_t(x, x)$, or $p_t(x, x)$, for fixed $x \in M$, as a function of $t \rightarrow +\infty$, with the geometry at infinity of M ?

By geometry at infinity we mean essentially volume growth and isoperimetric type properties. The connection with the decay of the heat kernel will be made through a scale of Sobolev inequalities, which incorporates the relevant geometric informations. These informations are much more robust than curvature assumptions.

Suppose one has identified classes of manifolds where the heat kernel behaves more or less as it does in the Euclidean spaces. Then another question one can ask is which part of real analysis (boundedness of Riesz transforms, H^1 - BMO duality) can be performed on such manifolds.

The same questions can be asked in a discrete setting, i.e. for random walks on graphs, see the survey [14]. Note that there one has to face a lot of additional difficulties, especially if one deals with discrete time.

In fact, one can connect directly the behaviour of the heat kernel on a manifold with the behaviour of random walks on a discrete skeleton via some discretisation techniques. There are results on heat kernels on manifolds that, up to now, can only be obtained in this way (see [21], Theorem 8 and [13], §VI). We won't develop this matter here, we refer the reader to [37], [52], [6], [10], [22], [13] and the references therein.

There exist already several (longer) surveys on heat kernels on non-compact manifolds, for example [48]. The one by Grigor'yan ([33]) is very informative and close in spirit to the present one. Grigor'yan recently wrote another quite interesting survey ([34]), which is however less oriented towards estimates of the heat kernel. Another possible complement to the present paper is [12].

In the last fifteen years, this field has undergone an important development and one cannot hope to give a comprehensive approach in a few pages, nor to quote all relevant papers. What follows is nothing but a subjective and partial account.

In §2, we shall explain why the control of the heat kernel decay is intermediate between an isoperimetric inequality and a volume lower bound, at least in a polynomial scale. In §3, we shall see that all three properties are in general different, but coincide for Lie groups or manifolds with non-negative curvature. In §4, we shall consider, among manifolds with the doubling property, the ones that satisfy Euclidean type estimates of the heat kernel, and we shall state real analysis properties for them, such as the bound-

edness of Riesz transforms and $H^1 - BMO$ duality. In §4, we shall characterise very general on-diagonal upper bounds for the heat kernel in terms of suitable L^2 isoperimetric inequalities. In §5, we shall give sufficient conditions for on-diagonal lower bounds.

2. The basic picture

It is essentially due to Varopoulos, around 1984, 85 ([49], [50], [51]), and may be summarised as follows:

$$\begin{array}{c}
 V(x, r) \geq C_1 r^D, \forall x \in M, r > 0 \\
 \updownarrow \\
 \|f\|_{\frac{2D}{D-2}} \leq C_2 \|\nabla f\|_2, \forall f \in \mathcal{C}_0^\infty(M) \iff \sup_{x \in M} p_t(x, x) \leq C_3 t^{-D/2}, \forall t > 0 \\
 \updownarrow \\
 |\Omega|^{\frac{D-1}{D}} \leq C_4 |\partial\Omega|, \forall \Omega \subset\subset M.
 \end{array}$$

Here $V(x, r)$ denotes the Riemannian volume of the geodesic ball $B(x, r)$ of center x and radius r . The L^p norms are taken with respect to the Riemannian measure, and ∇ is the Riemannian gradient. If Ω is a compact domain in M with smooth boundary (this is the meaning of $\Omega \subset\subset M$), $\partial\Omega$, $|\Omega|$ denotes its volume and $|\partial\Omega|$ the superficial measure of its boundary.

Remarks.

– To write down the Sobolev inequality, one has to assume that $D > 2$; this limitation is not serious, one can always write instead the Nash inequality

$$\|f\|_2^{1+\frac{2}{D}} \leq C \|f\|_1^{\frac{2}{D}} \|\nabla f\|_2, \forall f \in \mathcal{C}_0^\infty(M),$$

(see [3], where a systematic use of such inequalities was introduced). When $D > 2$, these two inequalities are equivalent (see [1], [27]) and we shall see in section 4 below that finally the Nash inequalities are more adapted to the treatment of non-polynomial volume growth situations.

– Provided one considers a manifold with a reasonably uniform local geometry, all the properties we consider can be localised at infinity, i.e. restricted for large time and large space, and then the relationship between them remains the same. This can be done through the discretisation techniques of [37], [6], [10], [22]. If one does not perform such a localisation, all the above inequalities can be valid only if $D \geq n$, where n is the topological dimension of M .

In the rest of this section, we shall sketch the proof of the implications that hold in the basic picture.

The two bottom-top vertical arrows are easy: the co-area formula shows that

$$|\Omega|^{\frac{D-1}{D}} \leq C_4 |\partial\Omega|, \forall \Omega \subset M, \text{ compact with smooth boundary}$$

is equivalent to

$$\|f\|_{\frac{D}{D-1}} \leq C_4 \|\nabla f\|_1, \forall f \in \mathcal{C}_0^\infty(M).$$

This inequality applied to $f^{\frac{2(D-1)}{D-2}}$ together with Hölder gives the L^2 Sobolev inequality. We shall see in section 3 below that conversely, the L^2 Sobolev inequality does not imply in turn the corresponding isoperimetric inequality.

Assume now that the Sobolev inequality holds, and apply it to a \mathcal{C}^∞ approximation of the tent function

$$f(x) = (r - d(x, x_0))_+,$$

where $x_0 \in M$ is fixed. Since $|\nabla f| = 1$ on $B(x_0, r)$, 0 elsewhere, and $f \geq r/2$ on $B(x_0, r/2)$, one gets

$$\frac{r}{2} V(x_0, r/2)^{\frac{D-2}{2D}} \leq C V(x_0, r), \forall x_0 \in M, r > 0.$$

An iteration argument yields then

$$V(x_0, r) \geq cr^D.$$

This is due to G. Carron ([4], [5]).

The horizontal arrow is due to Varopoulos ([49]), and it was the starting point of the whole subject. It relies on an abstract semi-group theorem. If e^{-tA} is symmetric submarkovian (but this can be weakened considerably, see [7], [8]), then

$$\|e^{-tA}\|_{1-\infty} \leq Ct^{-D/2} \iff \|f\|_{\frac{2D}{D-2}}^2 \leq C_2(Af, f), \forall f \in \mathcal{D}(A).$$

This gives the claimed equivalence because

$$\|e^{tA}\|_{1-\infty}' = \sup_{x \in M} p_t(x, x)$$

and

$$(-\Delta f, f) = \|\nabla f\|_2^2.$$

Let us give a trivial proof, taken from [8], of the implication from left to right. Replacing f by $e^{-sA}f$ in

$$\|f\|_{\frac{2D}{D-2}}^2 \leq C_2(Af, f)$$

gives

$$\|e^{-sA}f\|_{\frac{2D}{D-2}}^2 \leq \frac{-C_2}{2} \frac{d}{ds} \|e^{-sA}f\|_2^2.$$

Integrating between 0 and t yields, since e^{-sA} contracts the L^p spaces,

$$t\|e^{-tA}f\|_{\frac{2D}{D-2}}^2 \leq \int_0^t \|e^{-sA}f\|_{\frac{2D}{D-2}}^2 ds \leq \frac{C_2}{2} (\|f\|_2^2 - \|e^{-tA}f\|_2^2),$$

therefore

$$\|e^{-tA} f\|_{2-\frac{2D}{D-2}} \leq C' t^{-1/2}, \quad \forall t > 0.$$

Now an extrapolation lemma due to the author and Yves Raynaud ([7], §II) gives

$$\|e^{-tA} f\|_{1-\infty} \leq C' t^{-D/2}.$$

The other implication was proved already in [49] as follows: one writes

$$A^{-1/2} = c \int_0^{+\infty} t^{-1/2} e^{-tA} dt,$$

and using the $L^p - L^q$ estimates on e^{-tA} , one shows that $A^{-1/2}$ is bounded from L^2 to $L^{\frac{2D}{D-2}}$. As we already said, the up-to-date approach goes rather from the (more general) decay to some (more general) Nash type inequalities (see [13] and section 5 below).

It is easy to see that $p_t(x, y) \leq \sqrt{p_t(x, x) p_t(y, y)}$, but one expects $p_t(x, y)$ to be much smaller when x, y are far apart. Indeed, there are now sophisticated techniques to obtain bounds on $p_t(x, y)$ from bounds on $p_t(x, x)$ and $p_t(y, y)$ even for fixed x, y ([25], [32]). By semigroups methods relying on a trick due to E.B. Davies [24], one can prove that

$$\sup_{x, y} p_t(x, y) \leq C t^{-D/2}, \quad t > 0$$

self-improves into

$$p_t(x, y) \leq C' t^{-D/2} \left(1 + \frac{d^2(x, y)}{t}\right)^{D/2} \exp\left(-\frac{d^2(x, y)}{4t}\right) \quad \forall x, y \in M, \quad t > 0.$$

This estimate is due to Davies and Pang ([26]). For a simple proof, see [9]; this paper is aimed at the case of heat kernels on Lie groups, but the proof goes over to abstract submarkovian semigroups. Contrary to what one thought a few years back, the above estimate is not sharp, and can be slightly improved (see [47]).

Notice that the basic picture is not adapted to non-polynomial growth situations and says nothing about lower bounds of the heat kernel.

3. Volume growth and isoperimetry

Let us now concentrate on the two top-bottom negative arrows in the basic picture.

1. There exist manifolds such that $V(x, r) \geq cr^D$, $r > 0$ but where the inequality $\sup_{x \in M} p_t(x, x) \leq C t^{-D/2}$, $t > 0$, is false.

The example is due to Varopoulos in [54]. Take a Euclidean strip, and glue it smoothly with two half hyperbolic half-planes. The resulting manifold obviously has

uniform exponential growth, but it is conformal to the Euclidean plane, therefore it is recurrent. This very interesting but somewhat mysterious example is studied further in [18]. Also, one can ask what happens if the volume is really polynomial, i.e. $cr^D \leq V(x, r) \leq Cr^D$. The answer is also given in [18], see §6 below.

2. There exist manifolds such that $\sup_{x \in M} p_t(x, x) \leq Ct^{-D/2}$, $t > 0$, but $|\Omega|^{\frac{D-1}{D}} \leq C_4 |\partial\Omega|$, $\forall \Omega \subset M$, compact with smooth boundary is false.

Assume that

$$\sup_{x \in M} p_t(x, x) \leq Ct^{-D/2}, t > 0.$$

This upper estimate does imply an isoperimetric inequality for large sets, but for a weaker exponent. Indeed, it is equivalent to the Sobolev inequality

$$\|f\|_{\frac{2D}{D-2}} \leq C_2 \|\nabla f\|_2, \forall f \in \mathcal{C}_0^\infty(M).$$

Assume that M has a reasonably uniform local geometry (for example positive injectivity radius and Ricci curvature bounded from below, but much less is required, see [22]). Then the same inequality holds on a discretisation X of M ([37]), i.e.

$$\|f\|_{\frac{2D}{D-2}}^2 \leq C \|\nabla f\|_2^2 = \sum_{x, y \in X, x \sim y} |f(x) - f(y)|^2, \forall f \in \mathcal{C}_0(X).$$

Now taking $f = 1_\Omega$ yields

$$|\Omega|^{\frac{D-2}{D}} \leq C |\partial\Omega|,$$

where $\partial\Omega = \{x \in \Omega; \exists y \in \Omega^c, y \sim x\}$.

This discrete inequality can be brought back on M and gives the isoperimetric inequality $|\Omega|^{\frac{D'-1}{D'}} \leq C |\partial\Omega|$, where Ω ranges over the compact subsets of M with smooth boundary containing a geodesic ball of fixed radius (this is what Chavel and Feldman call a modified isoperimetric inequality, see [6]), with $D' = D/2$. Note that the greater D' , the better the isoperimetric inequality for large sets; on the other hand, if M has bounded geometry and, say, topological dimension D , then for small sets Ω , the inequality $|\Omega|^{\frac{D'-1}{D'}} \leq C |\partial\Omega|$ can hold only if $D' \geq D$.

This easy isoperimetric inequality is in fact all what one can get in general, as it was shown in [20].

THEOREM 3.1. — *For every integer $D \geq 6$ and every real $D' > D/2$, there exists a D -dimensional Riemannian manifold M with bounded sectional curvature and positive injectivity radius such that*

$$i) \sup_{x, y \in M} p_t(x, y) = O(t^{-D/2}), t \rightarrow +\infty,$$

ii) the isoperimetric inequality $|\Omega|^{\frac{D'-1}{D'}} \leq C |\partial\Omega|$, where Ω ranges over the compact subsets of M with smooth boundary containing a geodesic ball of fixed radius, is false.

The above result was improved by Carron in his thesis ([4]): he builds a manifold such that (i) holds and the estimate in (ii) is false for every $D' > D/2$.

These examples are rotationally invariant manifolds, with some narrow parts that destroy the isoperimetry, but do not affect too much the heat flow.

We can sum up what has been seen so far by saying that, at least in the polynomial scale, **the isoperimetric inequality controls from above the decay of the heat kernel, which in turn controls from below the volume growth, but the converses are false.**

There are however interesting situations where one can close the circle, namely where

$$V(x, r) \geq c r^D, \forall r > 0$$

implies

$$|\Omega|^{\frac{D-1}{D}} \leq C_4 |\partial\Omega|, \forall \Omega \subset M, \text{ compact with smooth boundary.}$$

These situations are the following:

- Manifolds with non-negative Ricci curvature (this was announced in [51], and can be seen by using the Li-Yau gradient estimates of [38]),
- Lie groups (or discrete groups) with polynomial volume growth ([53]).

There is a unifying principle behind these phenomena, that allows one to treat more general situations and also to go beyond the polynomial scale.

DEFINITION 3.2. — Denote $f_r(x) = \frac{1}{V(x, r)} \int_{B(x, r)} f(y) dy$. We say that M satisfies the pseudo-Poincaré inequality (PP_1) if

$$\|f - f_r\|_1 \leq Cr \|\nabla f\|_1, \forall f \in \mathcal{C}_0^\infty(M), r > 0.$$

The following theorem is due to Laurent Saloff-Coste and the author ([21]).

THEOREM 3.3. — Suppose (PP_1) and $V(x, r) \geq V(r)$, where V is strictly increasing to infinity. Then, there exist $c, C > 0$ such that

$$\frac{|\Omega|}{V^{-1}(c|\Omega|)} \leq C |\partial\Omega|,$$

for every Ω compact subset of M with smooth boundary.

Proof. — Write

$$\mu\{|f| \geq \lambda\} \leq \mu\{|f - f_r| \geq \lambda/2\} + \mu\{|f_r| > \lambda/2\}.$$

Since

$$\|f_r\| \leq \frac{\|f\|_1}{V(x, r)},$$

for $r_0 = V^{-1} \left(\frac{2\|f\|_1}{\lambda} \right)$ one has $\mu\{|f_{r_0}| > \lambda\} = 0$, and

$$\mu\{|f| \geq \lambda\} \leq \mu\{|f - f_{r_0}| \geq \lambda/2\} \leq \frac{2}{\lambda} \|f - f_{r_0}\|_1.$$

Now

$$\|f - f_{r_0}\|_1 \leq r_0 \|\nabla f\|_1$$

by (P_1) , and one gets

$$\mu\{|f| \geq \lambda\} \leq \frac{2}{\lambda} V^{-1} \left(\frac{2\|f\|_1}{\lambda} \right) \|\nabla f\|_1.$$

Taking $\lambda = 1$ and f a smooth approximation of 1_Ω gives the claim.

Now, when does (P_1) hold?

1. If M satisfies the doubling property

$$(D) \quad V(x, 2r) \leq CV(x, r), \forall x \in M, r > 0$$

and if the following family of Poincaré inequalities holds:

$$(P_1) \quad \int_{B(x,r)} |f - f_r(x)| \leq Cr \int_{B(x,Cr)} |\nabla f|, \forall x \in M, r > 0$$

therefore on manifolds with non-negative Ricci curvature (but also on manifolds with a reasonably uniform local geometry that are roughly isometric to manifolds with non-negative Ricci curvature, see [22]).

2. On Lie groups of polynomial or exponential volume growth (see [21], §1). The same theory works for finitely generated groups, again whatever the volume growth.

Theorem 3.3 also applies for co-compact coverings, see [21], §4. There, it is not clear whether (P_1) holds or not. But the fact that it holds on the deck transformation group suffices by discretisation.

Examples. — If $V(x, r) \geq r^D$ and (P_1) holds, one gets the classical Euclidean type inequality

$$|\Omega|^{\frac{D-1}{D}} \leq C|\partial\Omega|.$$

If $V(x, r) \geq c e^{cr}$ and (P_1) holds, one gets

$$\frac{|\Omega|}{\log |\Omega|} \leq C|\partial\Omega|.$$

The latter inequality is sharp; indeed, C. Pittet showed in [39] that on all polycyclic Lie groups with exponential growth, there exists a sequence of sets Ω_n whose volume tends to infinity such that

$$\frac{|\Omega_n|}{\log |\Omega_n|} \geq c |\partial \Omega_n|$$

(in fact, he is now able to prove the same fact on any solvable Lie group with exponential growth).

Note that the isoperimetric inequality of Theorem 3.3 implies the following L^2 version, called Faber-Krahn inequality (such inequalities were introduced in [30]):

$$\frac{c}{\varphi^2(c|\Omega|)} \leq \lambda_1(\Omega),$$

where φ is the reciprocal volume growth function V^{-1} .

So far we have encountered two Sobolev type inequalities associated with an exponent D : the L^1 inequality

$$\|f\|_{\frac{D}{D-1}} \leq C \|\nabla f\|_1, \forall f \in \mathcal{C}_0^\infty(M),$$

and the L^2 inequality

$$\|f\|_{\frac{2D}{D-2}} \leq C \|\nabla f\|_2, \forall f \in \mathcal{C}_0^\infty(M).$$

We also dealt with the property

$$V(x, r) \geq cr^D.$$

It is natural to consider the latter estimate as an L^∞ Sobolev inequality. Let us call these inequalities (S_D^1) , (S_D^2) and (S_D^∞) . One can fill in the gaps, and write down a complete scale of Sobolev inequalities for $1 \leq p \leq +\infty$. For example for $1 \leq p < D$, (S_D^p) will be

$$\|f\|_{\frac{pD}{D-p}} \leq C_p \|\nabla f\|_p, \forall f \in \mathcal{C}_0^\infty(M),$$

and for $D < p < +\infty$,

$$\|f\|_\infty \leq C_p \|f\|_p^{1-\frac{D}{p}} \|\nabla f\|_p^{\frac{D}{p}}, \forall f \in \mathcal{C}_0^\infty(M).$$

What is more interesting is that they can take the same form for all $p \in [1, +\infty]$, namely

$$\|f\|_p \leq C_p |\Omega|^{1/D} \|\nabla f\|_p, \forall f \in \mathcal{C}_0^\infty(\Omega)$$

(see [11], [12]). Behind this, there is a general principle that all reasonable forms of Sobolev inequality associated with a dimension D and an exponent p are equivalent (see [1]). One advantage of the above reformulation is that the dependences on p and on D are completely split. Also, it is tempting to interpret $|\Omega|^{1/D}$ as $\varphi(|\Omega|) = V^{-1}(|\Omega|)$ and to write the more general scale of inequalities

$$(S_\varphi^p) \quad \|f\|_p \leq C_p \varphi(|\Omega|) \|\nabla f\|_p, \forall f \in \mathcal{C}_0^\infty(\Omega).$$

Again, (S_φ^1) is equivalent to

$$\frac{|\Omega|}{\varphi(|\Omega|)} \leq C|\partial\Omega|,$$

(S_φ^∞) is equivalent to

$$V(x, r) \geq c\varphi^{-1}(r),$$

and (S_φ^2) is equivalent to the Faber-Krahn inequality

$$\frac{c}{\varphi^2(|\Omega|)} \leq \lambda_1(\Omega).$$

Also, (S_φ^p) implies (S_φ^q) for $1 \leq p < q < +\infty$. We shall see in §5 below that (S_φ^2) is equivalent to an upper bound of the heat kernel. At this point, we shall therefore have reached a full generalisation of the basic picture to non-polynomial volume growths.

Note that, contrary to the polynomial scale, (S_φ^2) does not imply any more (S_φ^∞) : there are heat kernel decays that are more rapid than one could predict from the volume growth. Indeed, in [40], Pittet and Saloff-Coste construct for any $n \in \mathbb{N}^*$ manifolds with exponential volume growth whose heat kernels behaves like $e^{-ct^{\frac{n}{n-2}}}$ (the typical "good" behaviour for exponential growth is $e^{-ct^{\frac{1}{2}}}$, whereas e^{-ct} corresponds to manifolds with a spectral gap).

Pseudo-Poincaré enables one to go down from (S_φ^∞) in the scale: for $1 \leq p < +\infty$, define

$$(PP_p) \quad \|f - f_r\|_p \leq Cr \|\nabla f\|_p, \quad \forall f \in \mathcal{C}_0^\infty(M), \quad r > 0.$$

Then (S_φ^∞) together with (PP_p) implies (S_φ^p) , see [12].

If one comes back to the polynomial scale, assuming (S_D^∞) i.e. $V(x, r) \geq cr^D$, then the Poincaré inequalities allow to get stronger Sobolev inequalities from the scale (S_D^p) . Indeed, if M satisfies (D) and

$$(P_p) \quad \begin{cases} \forall f \in \mathcal{C}_0^\infty(M), \quad \forall x \in M, \quad r > 0, \\ \int_{y \in B(x, r)} |f(y) - f_r(x)|^p dy \leq Cr^p \int_{B(x, Cr)} |\nabla f(y)|^p dy, \end{cases}$$

then for $1 < p < D$, one gets the global Sobolev inequality

$$\|f - c(f)\|_{\frac{Dp}{D-p}} \leq C \|\nabla f\|_p,$$

for all $f \in \mathcal{C}^\infty(M)$ such that $\|\nabla f\|_p < +\infty$, where $c(f)$ is some number depending on f (see [45]), and for $p > D$ the Lipschitz embedding

$$|f(x) - f(y)| \leq C d(x, y)^{1-\frac{D}{p}} \|\nabla f\|_p, \quad \forall f \in \mathcal{C}_0^\infty(M), \quad \forall x, y \in M$$

(see [11] where the case $p = D$ is also treated).

Note that the inequalities (P_D) (where D is the topological dimension and/or the volume growth exponent) play a role in the topic of quasi-conformal mappings between manifolds (see [36] and [23]) and that, if $cr^D \leq V(x, r) \leq Cr^D$, a characterisation of (P_p) can be obtained for $D - 1 < p < +\infty$ in terms of a new distance on M defined by means of the L^p norm of the gradient (see [19]).

4. Analysis on manifolds with regular volume growth

After the pioneering work by Li and Yau which gave the behaviour of the heat kernel on manifolds with non-negative Ricci curvature, the question was to understand the heat diffusion under more robust assumptions, that would be for instance stable under quasi-isometries. The two papers [44] and [29] gave an essentially complete answer for manifolds with the doubling property.

One says that M has regular volume growth, or satisfies the doubling property, if there exists C such that

$$(D) \quad V(x, 2r) \leq C V(x, r), \quad \forall x \in M, r > 0.$$

One says that M satisfies a relative Faber-Krahn inequality (see [29]) if there exists $c > 0, \nu > 0$ such that, for every $x \in M, r > 0$, and for every measurable subset Ω of M with positive measure contained in $B(x, r)$,

$$(FK) \quad \lambda_1(\Omega) \geq \frac{c}{r^2} \left(\frac{V(x, r)}{|\Omega|} \right)^\nu.$$

Finally one says that M satisfies the Poincaré inequality if there exists $C > 0$ and $C' \geq 1$ such that

$$(P) \quad \begin{cases} \forall f \in \mathcal{C}_0^\infty(M), \forall x \in M, r > 0, \\ \int_{y \in B(x, r)} |f(y) - f_r(x)|^2 dy \leq Cr^2 \int_{B(x, C'r)} |\nabla f(y)|^2 dy, \end{cases}$$

where

$$f_r(x) = \frac{1}{V(x, r)} \int_{B(x, r)} f(y) dy$$

(in the notation of section 4, (P) is nothing but (P_2)). The relationship between the above three properties is the following: (FK) implies (D) , and, together with (D) , (P) implies (FK) . This is explained for example in [17], §2.

Among manifolds satisfying (D) , (FK) and (P) characterise some heat kernel estimates.

THEOREM 4.1. — *Let M be a complete Riemannian manifold satisfying (D). Then the upper on-diagonal estimate*

$$p_t(x, x) \leq \frac{C}{V(x, \sqrt{t})}, \quad \forall t > 0, x \in M$$

is equivalent to (FK). If (FK) holds, one has in fact

$$p_t(x, y) \leq \frac{C}{V(x, \sqrt{t})} \exp\left(-\frac{d^2(x, y)}{Ct}\right), \quad \forall t > 0, x, y \in M.$$

It is easy to see that together with (D), the upper Gaussian estimate of $p_t(x, y)$ implies the on-diagonal estimate

$$p_t(x, x) \geq \frac{c}{V(x, \sqrt{t})}, \quad \forall t > 0, x \in M.$$

The off-diagonal lower estimate requires more.

THEOREM 4.2. — *Let M be a complete Riemannian manifold satisfying (D) and (P). Then*

$$\begin{aligned} \frac{c}{V(x, \sqrt{t})} \exp\left(-\frac{d^2(x, y)}{ct}\right) &\leq p_t(x, y) \\ &\leq \frac{C}{V(x, \sqrt{t})} \exp\left(-\frac{d^2(x, y)}{Ct}\right), \quad \forall t > 0, x, y \in M. \end{aligned}$$

Theorem 4.1 is due to Grigor'yan ([29]); Theorem 4.2 was also obtained by Grigor'yan in the same paper, and independently by Saloff-Coste ([43], [44]). In fact, both authors deduce from (D) and (P) a parabolic Harnack inequality that is equivalent to the upper and lower Gaussian estimate of the heat kernel. Saloff-Coste proves in addition that conversely, these estimates imply (D) and (P). For all this, see also the survey [46].

It is very easy to build manifolds that satisfy (FK), therefore (D), but not (P); take for instance \mathbb{R}^n without the unit ball, glue smoothly two copies of this manifold with boundary along the unit circle. The resulting manifold, call it $\mathbb{R}^n \amalg \mathbb{R}^n$, satisfies therefore all the above heat kernel estimates except for the off-diagonal lower bound.

Contrary to the Li-Yau gradient estimates, the parabolic Harnack inequality provides no pointwise upper bounds for the gradient of the heat kernel. However, integrated upper bounds for the gradient follows from the bounds on the heat kernel itself ([31]); together with a new theorem on singular integrals due to Duong and McIntosh ([28]), this is enough to get the boundedness of the Riesz transforms. The following theorem is proved in [15].

THEOREM 4.3. — *Let M be a complete Riemannian manifold satisfying the doubling volume property and such that*

$$p_t(x, x) \leq \frac{C}{V(x, \sqrt{t})}, \quad \forall t > 0, x \in M.$$

Then the Riesz transform $T = \nabla(-\Delta)^{-1/2}$ is weak $(1, 1)$, and bounded on L^p , $1 < p \leq 2$. That is, there exists C_p , $1 \leq p \leq 2$, such that, $\forall f \in \mathcal{C}_0^\infty(M)$,

$$\|\nabla f\|_p \leq C_p \|(-\Delta)^{1/2} f\|_p, \quad 1 < p \leq 2,$$

and

$$\|\nabla f\|_{1,\infty} \leq C_1 \|(-\Delta)^{1/2} f\|_1.$$

The above theorem admits a local version.

THEOREM 4.4. — *Let M be a complete Riemannian manifold satisfying the local doubling volume property*

$$\forall r_0 > 0, \exists C_{r_0} \text{ such that } V(x, 2r) \leq C_{r_0} V(x, r), \quad \forall x \in M, r \in]0, r_0[,$$

and whose volume growth at infinity is at most exponential in the sense that

$$V(x, \theta r) \leq C e^{c\theta} V(x, r), \quad \forall x \in M, \theta > 1, r \leq 1.$$

Suppose that

$$p_t(x, x) \leq \frac{C'}{V(x, \sqrt{t})},$$

for all $x \in M$ and $t \in]0, 1]$. Then there exists C_p , $1 \leq p \leq 2$, such that, $\forall f \in \mathcal{C}_0^\infty(M)$,

$$\|\nabla f\|_p \leq C_p \left(\|(-\Delta)^{1/2} f\|_p + \|f\|_p \right), \quad 1 < p \leq 2,$$

and

$$\|\nabla f\|_{1,\infty} \leq C_1 \left(\|(-\Delta)^{1/2} f\|_1 + \|f\|_1 \right).$$

By the same token, one can also treat manifolds with negative curvature. Indeed, a spectral gap suffices, together with small time estimates of the heat kernel and doubling for small radii. This gives an easy proof of some results by Lohoué.

THEOREM 4.5. — *Let M be a complete Riemannian manifold such that*

$$V(x, 2r) \leq C V(x, r), \quad \forall x \in M, r \in]0, 1[,$$

$$V(x, \theta r) \leq C e^{c\theta} V(x, r), \quad \forall x \in M, \theta > 1, r \leq 1,$$

and

$$p_t(x, x) \leq \frac{C'}{V(x, \sqrt{t})}, \quad \forall x \in M, t \in]0, 1].$$

Assume further that M has a spectral gap $\lambda > 0$:

$$\lambda \|f\|_2 \leq \|(-\Delta)f\|_2, \quad \forall f \in \mathcal{C}_0^\infty(M).$$

Then there exists C_p , $1 < p \leq 2$, such that,

$$\|\nabla f\|_p \leq C_p \|(-\Delta)^{1/2} f\|_p, \quad \forall f \in \mathcal{C}_0^\infty(M).$$

The previous theorems cover a much wider class of situations than what was previously known (see the references in [15] to the work of Lohoué, Bakry, Alexopoulos), but only for $1 \leq p \leq 2$, whereas all the known results covered the case $p > 2$. In fact, one cannot go further with the sole assumptions above.

Indeed, consider again $\mathbb{R}^n \coprod \mathbb{R}^n$, for $n = 2$. It has polynomial growth of exponent 2, and $p_t(x, x)$ is estimated from above and below by $\frac{1}{t}$, uniformly in x . Now, for $p > 2$, the Sobolev imbedding holds and says that

$$|f(x) - f(y)| \leq C_p d(x, y)^{1-\frac{2}{p}} \|\nabla f\|_p, \quad \forall f \in \mathcal{C}_0^\infty(M), \quad x, y \in M.$$

Assuming that

$$\|\nabla f\|_p \leq C \|(-\Delta)^{1/2} f\|_p,$$

and applying Sobolev to $p_t(x, \cdot)$, one would get an oscillation estimate on the heat kernel, therefore the off-diagonal lower bound (see [15] for details). But we already said that $\mathbb{R}^2 \coprod \mathbb{R}^2$ does not belong to the class of manifolds with (D) and (P).

If in addition M satisfies (P), then the operator $\nabla(-\Delta)^{-1/2}$ is in fact bounded from H^1 to L^1 . Also, the atomic H^1 space coincides with the space defined through the heat kernel, and as a consequence, the $H^1 - BMO$ duality holds. Again, $\mathbb{R}^2 \coprod \mathbb{R}^2$ is a counter-example. These results are due to E. Russ ([41], [42]). This was basically known for manifolds with non-negative Ricci curvature (see in particular the work of Bakry and the references in [41], [42]), but it is striking that one only needs proper heat kernel estimates.

5. Non-polynomial growth situations: Nash type inequalities and ultracontractivity

Another major breakthrough as far as heat kernel estimates are concerned was the paper [29] where the non-polynomial decays are treated for the first time in a completely satisfactory way. Previously, there had been the work of E.B. Davies (see [24] and the references therein), where one-parameter families of logarithmic Sobolev inequalities were used to characterise decays of the type

$$\|T_t\|_{1-\infty} \leq m(t),$$

for fairly general functions m and abstract Markov semigroups T_t . But first, logarithmic Sobolev are rather adapted to characterise hypercontractivity, i.e. an infinite dimensional phenomenon; this is why one has to parametrise them in order to capture ultracontractivity (this is another name for the fact that $\|e^{t\Delta}\|_{1-\infty}$ is finite for all t). It was thus natural to ask for a more direct route. Second, these logarithmic Sobolev inequalities have no clear isoperimetric interpretation.

In contrast, Grigor'yan shows, in the case of the heat kernel on a Riemannian manifold, that

$$\sup_{x \in M} p_t(x, x) \leq m(t)$$

if and only if

$$\lambda_1(\Omega) \geq \frac{1}{\varphi^2(|\Omega|)},$$

where the functions m and φ are deduced from one another by an explicit transformation.

In [13], one gives an abstract semigroup version of Grigor'yan's result. The advantage of this purely functional analytic proof is that it extends to discrete time and discrete space, i.e. random walks on graphs.

THEOREM 5.1. — *Let (X, ξ) be a σ -finite measure space and T_t a symmetric Markov semigroup on $L^2(X, \xi)$, with infinitesimal generator $-A$ and kernel p_t . Let m be a decreasing C^1 bijection of \mathbb{R}_+^* satisfying (δ) . Then*

$$\sup_{x \in X} p_t(x, x) \leq m(t), \quad \forall t > 0,$$

is equivalent to

$$\lambda_1(\Omega) \geq \frac{1}{\varphi^2(|\Omega|)},$$

for every Ω with finite measure in X , where m and φ are related by $-m'(t) = \frac{m(t)}{\varphi^2(1/m(t))}$.

The above equivalence is up to multiplicative constants: one identifies $m(\cdot)$ and $Cm(\cdot)$, $\varphi(\cdot)$ and $C\varphi(\cdot)$. Condition (δ) is a technical condition that affects the regularity of m but not its rate of decay.

In the above statement $\lambda_1(\Omega)$ is defined as $\inf_f \frac{(Af, f)}{\|f\|_2^2}$, where f ranges over the functions of $\mathcal{D}(A)$ supported in Ω . The Faber-Krahn type inequality (in other words (S_φ^2) in a geometric setting)

$$\lambda_1(\Omega) \geq \frac{1}{\varphi^2(|\Omega|)}$$

is equivalent to the Nash type inequality

$$\|f\|_1^2 \theta \left(\frac{\|f\|_2^2}{\|f\|_1^2} \right) \leq \operatorname{Re}(Af, f), \quad \forall f \in \mathcal{D}(A),$$

where $\theta(x) = \frac{x}{\varphi^2(1/x)}$ (see [1]).

It is interesting to note that the two implications in Theorem 5.1 have different sets of assumptions as far as T_t is concerned; to deduce the decay from the Nash inequality, one only needs a control of the $L^1 - L^1$ and $L^\infty - L^\infty$ norms, whereas to go back from the decay to Nash, one uses a symmetry assumption. This is no wonder; roughly speaking, the geometry of the underlying space governs all reasonable diffusions, including non-symmetric ones, but one cannot conclude from the behaviour of a diffusion to the geometry of the space unless the diffusion is symmetric (the influence of a drift could override the geometry!).

The first implication is contained implicitly or explicitly in the works of Nash, Carlen-Kusuoka-Stroock, Tomisaki (see the references in [13]).

PROPOSITION 5.2. — *Let T_t be a semigroup on $L^p(X, \xi)$, $1 \leq p \leq +\infty$, with infinitesimal generator $-A$. Suppose that T_t is equicontinuous on $L^1(X, \xi)$ and $L^\infty(X, \xi)$, i.e.*

$$\sup_t \|T_t\|_{1 \rightarrow 1}, \sup_t \|T_t\|_{\infty \rightarrow \infty} \leq M < +\infty,$$

and that

$$\theta(\|f\|_2^2) \leq \operatorname{Re}(Af, f), \quad \forall f \in \mathcal{D}(A), \quad \|f\|_1 \leq M,$$

where $\theta :]0, +\infty[\rightarrow]0, +\infty[$ is continuous and satisfies $\int_0^{+\infty} \frac{dx}{\theta(x)} < +\infty$. Then T_t is ultracontractive and

$$\|T_t\|_{1 \rightarrow \infty} \leq m(t), \quad \forall t > 0,$$

where m is the solution of

$$-m'(t) = \theta(m(t))$$

on $]0, +\infty[$ such that $m(0) = +\infty$, or alternatively the inverse function of $p(t) = \int_t^{+\infty} \frac{dx}{\theta(x)}$.

Note that if one puts together Proposition 5.2 and the fact that (S_φ^1) implies (S_φ^2) , one gets the following.

COROLLARY 5.3. — *Suppose that m and φ are as above. Then, if M satisfies the isoperimetric inequality*

$$\frac{|\Omega|}{\varphi(|\Omega|)} \leq C|\partial\Omega|,$$

for all compact domains Ω of M with smooth boundary, one has

$$\sup_{x \in X} p_t(x, x) \leq m(t), \quad \forall t > 0.$$

For a long time, unless m was a negative power, one did not know how to come back in an optimal way from the ultracontractivity estimate of a semigroup to a Nash or Sobolev type inequality. The methods of [51] and [3] induced a loss (see for example [51], §6). The only way was to use the one-parameter logarithmic Sobolev inequalities of Davies. However, it turned out that the converse is quite simple.

PROPOSITION 5.4. — *Let T_t be a symmetric contractive semigroup on L^2 , with infinitesimal generator $-A$, that satisfies*

$$\|T_t\|_{1 \rightarrow \infty} \leq m(t), \quad \forall t > 0.$$

Then

$$\tilde{\theta}(\|f\|_2^2) \leq (Af, f), \quad \forall f \in \mathcal{D}(A), \quad \|f\|_1 \leq 1,$$

where $\tilde{\theta}(x) = \sup_{t>0} \frac{x}{2t} \log \frac{x}{m(t)}$.

Sketch of proof: One starts with the following inequality, that can be proved by applying Jensen to the spectral resolution of A

$$\exp\left(-2\frac{(Af, f)}{\|f\|_2^2}t\right) \leq \frac{\|T_t f\|_2^2}{\|f\|_2^2}.$$

Now, by hypothesis, $\|T_t f\|_2^2 \leq m(t)\|f\|_1^2$. Fix $f \in \mathcal{D}(A) \setminus \{0\}$ such that $\|f\|_1 \leq 1$. One has

$$\exp\left(-2\frac{(Af, f)}{\|f\|_2^2}t\right) \leq \frac{m(t)}{\|f\|_2^2}, \quad \forall t > 0,$$

hence

$$\frac{(Af, f)}{\|f\|_2^2} \geq \frac{1}{2t} \log \frac{\|f\|_2^2}{m(t)}, \quad \forall t > 0.$$

This proves the Proposition.

Now a calculus lemma due to Grigor'yan proves that if m satisfies (δ) one can replace $\bar{\theta}$ by $\theta = -m' \circ m^{-1}$.

6. Lower bounds for the heat kernel

The only lower bounds on the heat kernel we have seen till now are obtained either as consequences of upper bounds, or at least at the same time than upper bounds. Also, (D) and (P) are very restrictive conditions, and one would like to have criteria than ensure lower bounds for manifolds with more rapid volume growth or without (P) . In [16], one derives sufficient conditions for on-diagonal lower bounds in terms of what we call anti-Faber-Krahn inequalities, without going through upper bounds.

THEOREM 6.1. — *Let m and φ be as in Theorem 5.1. Suppose that, for every $\xi \in \mathbb{R}_+^*$, there exists Ω_ξ such that $|\Omega_\xi| \leq \xi$ and $\lambda_1(\Omega_\xi) \leq \frac{1}{\varphi^2(\xi)}$. Then*

$$\sup_{x \in X} p_t(x, x) \geq m(ct), \quad \forall t > 0.$$

It is natural to ask whether anti-isoperimetry implies lower bounds on the heat kernel: suppose that, for every $\xi \in \mathbb{R}_+^*$, there exists Ω_ξ such that $|\Omega_\xi| \leq \xi$ and $|\partial\Omega_\xi| \leq \frac{\xi}{\varphi(\xi)}$. Can one get the same conclusion as in Theorem 6.1? Some partial results are given in [16], but the theory is not yet complete.

One can also get pointwise lower bounds for $p_t(x, x)$ from upper bounds on the volume growth.

PROPOSITION 6.2. — *Fix $x \in M$ and suppose that M has bounded geometry around x . Suppose that $V(x, r) \leq Cr^D$, $\forall r \geq 1$. Then*

$$p_t(x, x) \geq \frac{c}{(t \log t)^{D/2}}, \quad \forall t \geq 1,$$

and this bound is sharp.

Results for more general volume growths can be found in [16], §6.

Coming back to $\sup_x p_t(x, x)$, one may ask what is the range of possible behaviours, say when the volume is really polynomial, i.e. $cr^D \leq V(x, r) \leq Cr^D$. Using the above tools, one can give in this case a complete answer.

THEOREM 6.3. — *Let M a manifold with bounded geometry such that $V(x, r)$ satisfies $cr^D \leq V(x, r) \leq Cr^D$. Then*

$$c' t^{-\frac{D}{2}} \leq \sup p_t(x, x) \leq C' t^{-\frac{D}{D-1}},$$

and both bounds are sharp.

The lower bound is a consequence of [16], Theorem 2.7. It follows from the inequality

$$\sup_{x \in M} p_t(x, x) \geq \sup_{\Omega} \left\{ \frac{e^{-\lambda_1(\Omega)t}}{|\Omega|} \right\}$$

and from the fact that on a manifold that satisfies the doubling property

$$(D) \quad V(x, 2r) \leq CV(x, r), \quad \forall x \in M, r > 0,$$

one has

$$\lambda_1(B(x, r)) \leq \frac{C}{r^2}, \quad \forall x \in M, r > 0.$$

The upper bound comes from [21], Théorème 8, and uses discretisation.

The optimality of the lower bound is no mystery. The fact that there exists a manifold with exponential volume growth of exponent D and such that

$$\sup_{x \in M} p_t(x, x) \geq ct^{-\frac{D}{D-1}}$$

comes from [18], where more results are to be found on the connection between the volume growth alone and the heat kernel decay. In particular, it is proved there that in the example of Varopoulos quoted in §3, the behaviour of $\sup_x p_t(x, x)$ is close, up to a logarithm, to the maximum allowed for a non-compact manifold, i.e. $\frac{C}{\sqrt{t}}$.

Let us close this survey by making clear that many aspects of the large time heat kernel behaviour are largely unknown and still wait to be explored. Let us mention for instance off-diagonal bounds without (D) and (P), good estimates on manifolds with a spectral gap, and the study of the heat kernel on differential forms (see [2] for very preliminary results). See also [35] and [18] for some recent new directions.

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