HEAT KERNEL ON A NON-COMPACT RIEMANNIAN MANIFOLD

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Dedicated to E.M.Landis

0. Introduction

This paper is a survey of some recent results on the heat kernel of a non-compact complete Riemannian manifold. The fast progress during the last 10-15 years has turned this field into a well-developed theory which on the one hand has its own traditions and stimulations for further investigations and, on the other hand, is connected heavily with adjacent spheres of geometry, potential theory, partial differential equations, theory of operators, stochastic analysis etc. Of course, the size of this work is far from being enough to exhaust this topic: we refer the reader to books by I.Chavel [7] , B.Davies [20] , D.Robinson [58] , N.Varopoulos, L.Saloff-Coste and T.Coulhon [69] for a systematic account of properties of the heat kernel in different contexts.

In the present paper, we are mainly concerned with a new method for obtaining upper bounds of the heat kernel through geometry of the underlying space, mainly following the works of the author [30] - [28] . Let M be a smooth connected non-compact geodesically complete Riemannian manifold, Δ be the Laplace operator associated with the Riemannian metric, $n \geq 2$ be the dimension of M . The subject of this paper is the heat kernel $p(x, y, t)$ (where $x, y \in M, t > 0$) being by definition the smallest positive fundamental solution to the heat equation

$$u_t - \Delta u = 0$$

which is known to exist on any manifold (see [7]). From the probabilistic point of view, $p(x, y, t)$ is the transition density of the Brownian motion on the manifold. Other than being a fundamental solution, the heat kernel possesses the following general properties:

1° Symmetry: $p(x, y, t) = p(y, x, t)$, which reflects self-adjointness of the Laplace operator;

2° The semigroup property:

$$p(x, y, t) = \int_M p(x, z, \tau) p(z, y, t - \tau) dz, \ \forall x, y \in M, \ 0 < \tau < t$$

which gives rise to the semigroup theory;

3° The total probability does not exceed 1:

$$\int_M p(x, y, t) dy \leq 1.$$

We want to clarify the geometric dependence of the heat kernel, namely, how its behaviour for a large time t and for a large distance $r = \operatorname{dist}(x, y)$ depends on geometric properties of the manifold in question. Of course, it is possible to ask how the heat kernel behaves itself as $t \to 0$ but this is another story (see , for example, [50] , [7]). Our task is to connect a long time and long distance behaviour of the heat kernel with geometry "in the large" of the manifold.

Let us recall that in the Euclidean space $\mathbf{R}^n$ the heat kernel is given by the formula

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

while in the 3 -dimensional hyperbolic space $\mathbf{H}^3_k$ (of the constant sectional curvature $-k^2$) the heat kernel takes the form

$$p(x, y, t) = \frac{1}{(4\pi t)^{3/2}} \frac{kr}{\sinh(kr)} \exp\left(-\frac{r^2}{4t} - k^2 t \right) \quad . \tag{0.1}$$

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More generally, in the $n-$ dimensional hyperbolic space $\mathbf{H}^n_k$ the heat kernel is finitely proportional to the function

$$\frac{(1+r+t)^{\kappa-1}(1+r)}{t^{n/2}}\exp\left(-\frac{r^2}{4t}-\kappa^2k^2t-\kappa kr\right) \tag{0.2}$$

where $\kappa=(n-1)/2$ (see [17]).

It is unlikely that so sharp information about the heat kernel can be obtained in a general setting. One may anticipate only getting estimates depending on what is known about the geometry of the manifold.

The following questions form the framework of the paper.

1. *On which manifolds does the heat kernel satisfy for all $x,y\in M,t>0$ (or, at least for large t) the inequality*

$$p(x,y,t)\le\frac{\text{const}}{f(t)} \tag{0.3}$$

with a given increasing function $f(t)$?

For example, in $\mathbf{R}^n$ we may put

$$f(t)=t^{n/2}$$

and in the hyperbolic space $\mathbf{H}^n_k$

$$f(t)=\exp(ct)\ ,c=\kappa^2k^2$$

for a large t. There are examples of manifolds, namely, covering manifolds with a polycyclic deck transformation group (see [68]) for which the optimal function $f(t)$ has an intermediate growth between a polynomial and an exponential:

$$f(t)=\exp(ct^{\frac{1}{3}})\ ,c>0\ .$$

We shall present necessary and sufficient conditions for the inequality (0.3) to be true in terms of isoperimetric properties of the manifold.

2. *How to describe the behaviour of the heat kernel for a large r ?* We describe a new approach on how to involve the Gaussian term $\exp\left(-\frac{r^2}{ct}\right)$ in heat kernel estimates. The heart of the matter is that we study in a systematic manner the following integral of the heat kernel with the Gaussian weight:

$$E(x,t)=\int_M p^2(x,y,t)\exp\left(\frac{r^2}{Dt}\right)\,dy \tag{0.4}$$

where $r=\operatorname{dist}(x,y)$ and $D>2$ is a given constant. We obtain first estimates of the kind

$$E(x,t)\le\frac{\text{const}}{f(t)} \tag{0.5}$$

which enable us to pass to pointwise bounds of the heat kernel containing the Gaussian factor. It is surprising that this factor is not sensitive to geometry of the manifold albeit in most examples, it is responsible for the heat kernel behaviour as $r\to\infty$.

3. *How to estimate derivatives of the heat kernel ?* Our approach to estimate derivatives of the heat kernel is also based upon properties of integrals similar to (0.4) :

$$E_m(x,t)=\int_M\left|\nabla^m_y p\right|^2(x,y,t)\exp\left(\frac{r^2}{Dt}\right)\,dy$$

where $m=1,2,...$. The inequality (0.5) implies a similar estimate of $E_m(x,t)$ which in turn enables us to estimate pointwise the time derivatives of the heat kernel.

4. *Harnack inequality and double-sided estimates.* We state the criterion of validity of the Harnack inequality for the heat equation in terms of the Poincaré inequality and the doubling volume property and show which heat kernel estimates are deduced from it.

5. *To what extent it is possible to derive non-trivial information about the heat kernel using only local geometric information concerning the manifold ?* The point is that in order to get the inequality (0.3) one has to know isoperimetric properties of an arbitrary region including arbitrarily large regions or, in other words, to know global geometric properties of the manifold. By a local property of a manifold we mean one which depends only on intrinsic geometry of balls of a fixed (small) radius. For example, curvature is a local property but very often it is not an adequate hypothesis for heat kernel estimation - normally it suffices to know the Riemannian metric itself rather than its derivatives. We define in local geometric terms (not involving any derivatives of the metric) a class of manifolds which includes the manifolds of bounded geometry and which is very well suited to our main purpose - heat kernel estimations.

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1. On-diagonal estimates

This is the term to denote an estimate as (0.3) because it follows from the same inequality for $x = y$. It is now well-known and standard that a special case of (0.3) with the Euclidean function $f(t) = \mathrm{const}\, t^{n/2}$, namely, the on-diagonal estimate

$$p(x, y, t) \leq \frac{\mathrm{const}}{t^{n/2}} \tag{1.1}$$

is deduced from the Sobolev inequality: for any smooth function $v \in C_c^\infty(M)$

$$\int_M |\nabla v|^2 \geq c \, \|v\|^2_{\frac{2n}{n-2}} \ , \ c > 0 \tag{1.2}$$

where $\|v\|_k$ stands for

$$\left(\int_M |v|^k \right)^{1/k}$$

(of course we have to assume in (1.2) that $n > 2$).

A geometric background of the Sobolev inequality (1.2) is that it is close to the classical isoperimetric inequality between the volume of a bounded region $\Omega \subset M$ and the area of its boundary

$$\mathrm{Area}\,(\partial \Omega) \geq c \mathrm{Vol}\,(\Omega)^{(n-1)/n}, \tag{1.3}$$

namely, (1.3) implies (1.2) (see [49]). The converse is true provided the manifold has non-negative Ricci curvature but generally the Sobolev inequality is a weaker hypothesis than (1.3) (see [63] , [67] , [12] ,[10]).

Historically, the machinery for obtaining the estimate (1.1) was invented by Nash [55] for the case of elliptic operators in $\mathbf{R}^n$. He derived it from a functional inequality which is now referred to as *Nash's inequality* : for any $v \in C_c^\infty(M)$ such that $\|v\|_1 = 1$

$$\int_M |\nabla v|^2 \geq c \, \|v\|_2^{2+4/n} , \ c > 0 \tag{1.4}$$

and his method works also for the setting of manifolds and even in more general situations (see [5]). On the other hand, the Sobolev inequality (1.2) implies (1.4) upon a suitable application of a Hölder inequality whence we get the following implications:

$$\textit{Sobolev's inequality} \implies \textit{Nash's inequality} \implies \textit{on} - \textit{diagonal estimate}\ (1.1)$$

The next step is due to Varopoulos [63] who showed (in a more general context of abstract semigroups) that the Sobolev inequality (1.2) is not only sufficient but a necessary condition as well for the upper bound (1.1) to hold:

$$\textit{on} - \textit{diagonal estimate}\ (1.1) \implies \textit{Sobolev's inequality}$$

Therefore, all three inequalities under consideration are equivalent. Another proof of the fact that the Nash inequality is equivalent to (1.1) was given by Carlen, Kusuoka and Stroock [5] . Their proof has an additional benefit that it goes through also if $n \leq 2$ (in the general context of their work n is not necessarily a dimension).

Carlen, Kusuoka and Stroock were also able to modify the Nash inequality to consider heat kernel estimates separately for small and large time. Indeed, the fact, that in $\mathbf{R}^n$ on-diagonal behaviour of the heat kernel is described by the same power of t as $t \to 0$ and as $t \to \infty$ reflects the presence in $\mathbf{R}^n$ of the scale transformation. Even in a homogeneous hyperbolic space it is not so - as one sees from (0.1) or (0.2) the heat kernel decreases on the diagonal, $x = y$, for a small time as $\mathrm{const}\, t^{-n/2}$ and for a large time as $\exp(-ct)$.

The further progress in understanding of on-diagonal long time behaviour of the heat kernel is due to B.Davies [15] , [16] , [19] , [20] (see also bibliography in [20]). He proved that the on-diagonal estimate (0.3) with a more general function $f(t)$ can be derived from the following *log-Sobolev inequality* : for any $v \in C_c^\infty(M), v \geq 0$ such that $\|v\|_2 = 1$

$$\int_M v^2 \log v \leq \varepsilon \int_M |\nabla v|^2 + \beta(\varepsilon) \tag{1.5}$$

where the number ε is supposed to range $(0, +\infty)$ and $\beta(\varepsilon)$ is some decreasing function. In fact, the concrete form of the function $f(t)$ depends on $\beta(\varepsilon)$. Conversely, if one is given the on-diagonal estimate (0.3) then (1.5) follows where $\beta(\varepsilon)$ is expressed through $f(t)$. For example, if

$$f(t) = \begin{cases} t^{\nu/2} & , \ t \leq 1 \\ t^{\mu/2} & , \ t > 1 \end{cases}$$

where $\nu, \mu > 0$ then (0.3) is equivalent to the log-Sobolev inequality (1.5) where

$$\beta(\varepsilon) = \begin{cases} c - \frac{\nu}{4} \log \varepsilon & , \ 0 < \varepsilon \leq 1 \\ c - \frac{\mu}{4} \log \varepsilon & , \ 1 < \varepsilon < \infty \end{cases} .$$

A drawback of this method is that normally it is very difficult to verify directly a log-Sobolev inequality. We are going to describe another approach which covers all possible ways of decay of the heat kernel as $t \to \infty$ and establishes equivalence between the on-diagonal estimate (0.3) and some inequality of a Faber-Krahn type which we use in place of the Sobolev, Nash and log-Sobolev inequalities. So far this method is developed only in the context of the heat equation on manifolds but there is no doubt that it is applicable for general semigroups as the theorems cited above. The advantage of this approach is that it relates the heat kernel's on-diagonal behaviour to a very clear geometric object - the first Dirichlet eigenvalue of a region which has long been studied by geometers.

Actually, it is not surprising that the heat kernel is connected to Dirichlet eigenvalues. Indeed, if p_Ω denotes the heat kernel in a region Ω subject to the Dirichlet boundary condition then the eigenvalue expansion says that

$$p_\Omega(x, y, t) = \sum_{k=1}^{\infty} \exp(-\lambda_k(\Omega)t)\varphi_k(x)\varphi_k(y)$$

where $\lambda_k(\Omega)$ is the $k-$ th Dirichlet eigenvalue of Ω and φ_k is the corresponding eigenfunction so that $\{\varphi_k\}$ is an orthonormal basis in $L^2(\Omega)$. Since $\lambda_1(\Omega)$ is a simple eigenvalue, it follows that

$$p_\Omega(x, y, t) \sim \exp(-\lambda_1(\Omega)t) \quad t \to \infty .$$

Let $\Omega \to M$ denote an exhaustion of M by a sequence of regions Ω. Then we have $p_\Omega \to p$ and $\lambda_1(\Omega) \to \lambda_1(M)$ as $\Omega \to M$ where $\lambda_1(M)$ is the spectral gap of the Laplacian as an operator in $L^2(M)$ i.e. the bottom of the spectrum of $-\Delta$ (see [7]). If $\lambda_1(M) > 0$ as happens on the hyperbolic space then we can hope that p behaves as $\exp(-\lambda_1(M)t)$ as $t \to \infty$. For the case $\lambda_1(M) = 0$ it gives nothing but one can guess that the decay of p as $t \to \infty$ may depend upon how quickly $\lambda_1(\Omega)$ approaches to 0 as $\Omega \to M$.

This is our motivation of the following definition.

Definition 1 Let $\Lambda(v)$ be a positive continuous monotonically decreasing function in $(0, +\infty)$. We say that *a Λ-isoperimetric inequality* holds in a region $\Omega \subset M$, if for any pre-compact subregion $G \subset \Omega$, we have

$$\lambda_1(G) \geq \Lambda(\operatorname{Vol} G). \tag{1.6}$$

The following theorem is a realization of the idea above.

Theorem 1 *([31]) If a Λ-isoperimetric inequality holds on a manifold M then for all $x, y \in M, t > 0$ and for any $\delta \in (0, 1)$ the following heat kernel estimate is valid:*

$$p(x, y, t) \leq \frac{\text{const}_\delta}{V(\delta t)} \tag{1.7}$$

where the function $V(t)$ is defined by means of the following identity:

$$t = \int_0^{V(t)} \frac{dv}{v\Lambda(v)} \tag{1.8}$$

and we assume that the integral in (1.8) converges at 0.

Examples. 1. Let us set

$$\Lambda(v) = \text{const}\begin{cases} v^{-2/n} & , \; v \le 1 \\ v^{-2/m} & , \; v > 1 \end{cases}, \tag{1.9}$$

then by Theorem 1 we have the following estimate

$$p(x, y, t) \le \text{const}\begin{cases} t^{-n/2} & , \; t \le 1 \\ t^{-m/2} & , \; t > 1 \end{cases}. \tag{1.10}$$

It is well-known that in the Euclidean space a Λ-isoperimetric inequality holds with the function (1.9) where $m = n$. Therefore, (1.10) yields in this case simply the Euclidean estimate of the heat kernel. There are also interesting examples of manifolds with $m \neq n$. Indeed, if M is a direct product $K \times \mathbf{R}^m$ where K is a compact $(n-m)$ -dimensional manifold then it satisfies the hypotheses of Theorem 1 with the function (1.9) (see [25]) Here we have $m < n$. The case $m > n$ occurs if the manifold M covers a compact manifold with a polynomial deck transformation group (see the next example). Finally, for manifolds with bounded geometry we have always $m = 1$ which will be discussed in Section 5.

2. Let M cover a compact manifold K with a deck transformation group Γ and let $\gamma(r)$ be an increasing lower bound for the the volume of a combinatorial ball on Γ of the radius r (although the function $\gamma(r)$ need be defined only for integer values of r we suppose that it is actually defined for all $r > 0$, is continuous and, besides, $\gamma(1) = 2$). Let us introduce the function

$$g(v) = \begin{cases} v^{\frac{n-1}{n}} & , \; v \le 1 \\ \frac{v}{\gamma^{-1}(2v)} & , \; v > 1 \end{cases}$$

then by the theorem of Coulhon and Saloff-Coste [14] for any bounded region $\Omega \subset M$ with a smooth boundary we have the isoperimetric inequality:

$$\text{Area}\,(\partial\Omega) \ge c g(\text{Vol}\,\Omega), \;\; c > 0 \tag{1.11}$$

provided $\gamma(r)$ is one of the following functions

$$\gamma(r) = \text{const}\, r^m, \;\; m > 0 \tag{1.12}$$

or

$$\gamma(r) = \text{const}\, \exp(cr^\alpha), \;\; 0 < \alpha \le 1 \tag{1.13}$$

(apparently, $\gamma(r)$ may be a more general function but the theorem [14] treats only the two cases mentioned above). On the other hand as shown in [31] the isoperimetric inequality (1.11) implies the Λ-isoperimetric inequality (1.6) with the function

$$\Lambda(v) = \text{const}\left(\frac{g(v)}{v}\right)^2$$

which yields in this case

$$\Lambda(v) = \text{const}\begin{cases} v^{-2/n} & , \; v \le 1 \\ (\gamma^{-1}(2v))^{-2} & , \; v > 1 \end{cases}.$$

If we have a polynomial group Γ i.e. the volume function (1.12) then we get exactly the setting of the preceding example. For the case of superpolynomial volume growth (1.13) we get the function

$$\Lambda(v) = \begin{cases} \text{const}_1 v^{-2/n} & , \; v \le 1 \\ \text{const}_2 (\log 2v)^{-2/\alpha} & , \; v > 1 \end{cases} \tag{1.14}$$

and by Theorem 1 we have for large t

$$p(x, y, t) \le \text{const}\, \exp\left(-ct^{\frac{\alpha}{\alpha+2}}\right), \;\; c > 0.$$

In particular, if $\alpha = 1$ as takes place for the group Γ of an exponential volume growth then the heat kernel decreases for large t at least as fast as $\exp(-ct^{\frac{1}{3}})$.

The corresponding heat kernel bounds on a discrete group and on a group Lie were proved first by Varopoulos [68] .

3. Let

$$\Lambda(v) = \begin{cases} cv^{-2/n} & , \ v \le v_0 \\ \lambda & , \ v > v_0 \end{cases} \tag{1.15}$$

where the constant $\lambda > 0$ is nothing but the spectral gap $\lambda_1(M)$. The Λ-isoperimetric inequality with this function holds, for example, on a Cartan-Hadamard manifold (which follows from [37]) with a positive spectral gap. The estimate of Theorem 1 can in this case be slightly improved and gives

$$p(x, y, t) \le \frac{\text{const}}{\min(t^{n/2}, 1)} \exp(-\lambda t) \ . \tag{1.16}$$

We do not touch here on a more subtle estimate of the kind

$$p(x, y, t) \le \frac{\text{const}}{t^{\nu}} \exp(-\lambda t), \ t > 1, \ \nu > 0 \tag{1.17}$$

which is valid on the hyperbolic space and on symmetric spaces of rank 1 (see [4]) - Theorem 1 is too robust to catch the term t^{ν} if $\lambda > 0$. As was shown by J.Lunt [46] the factor t^{ν} in (1.17) can be removed by modifying locally the metric of the manifold. See also [11] for positive results.

Let us turn to a converse theorem starting with the observation that the function $V(t)$ obtained by (1.8) satisfies necessarily the following conditions:

(i) $V(t) \in C^1((0, +\infty))$ and $V'(t) > 0$ for all $t > 0$
(ii) $V(0) = 0, \ V(\infty) = \infty$
(iii) $\frac{V'(t)}{V(t)}$ is monotonically decreasing

where the last property follows from the identity

$$\Lambda(V(t)) = \frac{V'(t)}{V(t)} \tag{1.18}$$

which is nothing but (1.8) in another form. We shall impose on the function $V(t)$ an additional restriction.

Definition 2 We say that a decreasing function $\varphi(t)$ is of a polynomial decay if for some $\alpha > 0$ (which will be fixed in what follows) and for all $\beta \in [1, 2]$

$$\varphi(\beta t) \ge \alpha \varphi(t) \ .$$

Suppose that we are given a function $V(t)$ satisfying (i)-(iii) as well as the following hypothesis:

(iv) the function $\frac{V'(t)}{V(t)}$ is of polynomial decay.

The following theorem contains, in fact, a converse to Theorem 1.

Theorem 2 *([31]) Suppose that for all $x \in M$ and $t > 0$ we have the estimate:*

$$p(x, x, t) \le \frac{1}{V(t)}, \tag{1.19}$$

where the function $V(t)$ satisfies (i)-(iv) and let us define the function Λ by (1.18) . Then for any pre-compact open set $\Omega \subset M$ and any integer $k \ge 1$

$$\lambda_k(\Omega) \ge \text{const}_{\alpha} \Lambda\left(\frac{\operatorname{Vol}\Omega}{k}\right) \ . \tag{1.20}$$

In particular, for $k = 1$ we see that the on-diagonal estimate (1.19) implies const$\Lambda-$ isoperimetric inequality.

The regularity condition (iv) is not restrictive: at least such functions as

$$V(t) = \exp(t^{\nu}), \quad t^{\nu}, \quad (\log t)^{\nu}, \quad \nu > 0 \tag{1.21}$$

and their products satisfy (ıv) for large t. Hence, for such functions $V(t)$ the theorems 1,2 are converse up to constant multiples. If $V(t)$ does not satisfy (ıv) then some other Λ-isoperimetric inequality could be nevertheless deduced from (1.19) which would be, however, weaker than (1.20) .

We encountered in some of our considerations with a necessity to impose some regularity assumptions on a function which is responsible for the heat kernel decay in time. In all the cases these restrictions arose for technical reasons but, apparently, they are deeply rooted in the fact that the heat kernel $p(x,x,t)$ is a regular enough function in t. For example, on any manifold $\log p(x,x,t)$ is a concave decreasing function of t. It would be interesting to describe explicitly the class of all functions $p(x,x,\cdot)$ varying the manifold and the point x.

One of the possible consequences of Theorems 1,2 is that a Λ-isoperimetric inequality implies a similar inequality (1.20) for the higher eigenvalues.

Let us observe also that Theorems 1,2 imply that the Euclidean heat kernel estimate (1.1) is equivalent to the Faber-Krahn type inequality

$$\lambda_1(\Omega) \geq \operatorname{const} (\operatorname{Vol}\Omega)^{-2/n} \ . \tag{1.22}$$

Therefore, (1.22) is equivalent to both Sobolev's and Nash's inequality. This was shown also directly by Carron [6] .

The heart of the proof of Theorem 1 in [31] is the following lemma.

Lemma *The Λ-isoperimetric inequality (1.6) implies that for any function $v \in C_c^\infty(M)$, $v \geq 0$ such that $\|v\|_1 = 1$ and for any $\delta \in (0,1)$*

$$\int_M |\nabla v|^2 \geq (1-\delta)\, \|v\|_2^2 \, \Lambda\left(\frac{2}{\delta} \|v\|_2^{-2} \right) \ . \tag{1.23}$$

The heat kernel estimate (1.7) follows from (1.23) in a standard manner by deriving a differential inequality for $p(x,x,2t) \equiv \int p^2(x,y,t)dy$ as a function of t with subsequent integration of it.

Let us observe that the inequality (1.23) takes the form of Nash's inequality (1.4) if the Λ-isoperimetric inequality is the Euclidean one (1.22) . Hence, (1.23) can be regarded as an extension of the Nash inequality. Apparently, inequalities similar to (1.23) appeared first in works of A.Gushchin (see [35] , [36] and references therein) devoted to parabolic equations in unbounded domains of $\mathbf{R}^n$.

To conclude the discussion around theorems 1,2 let us record the fact that under the conditions (ı)-(ıv) the following three hypotheses are equivalent (up to constant factors):

- the Λ-isoperimetric inequality (1.6)
- Nash type inequality (1.23)
- on-diagonal upper bound (1.19)

provided the functions $\Lambda(v)$ and $V(t)$ are connected by (1.8) or (1.18) .

2. The weighted integral of the heat kernel

The following statement makes clear the role of the quantity

$$E(x,t) = \int_M p^2(x,y,t) \exp\left(\frac{r^2}{Dt} \right) dy \tag{2.1}$$

where $r = \operatorname{dist}(x,y)$ and the constant $D > 2$ is considered as given.

Theorem 3 *([31]) On an arbitrary manifold M and for any $x \in M$ the function $E(x,t)$ is a finite continuous decreasing function of t. Furthermore, the following inequality holds for all $x,y \in M$ and $t > 0$*

$$p(x,y,t) \leq \exp\left(-\frac{r^2}{2Dt} \right) \sqrt{E(x,\frac{t}{2})E(y,\frac{t}{2})} \tag{2.2}$$

where $r = \operatorname{dist}(x,y)$.

Moreover, if $\lambda = \lambda_1(M)$ is the spectral gap of the Laplacian then $E(x,t)\exp(\lambda t)$ is a decreasing function of t and

$$p(x,y,t) \leq \exp\left(-\frac{r^2}{2Dt} - \lambda t \right) \exp(\lambda t_0) \sqrt{E(x,\frac{t_0}{2})E(y,\frac{t_0}{2})} \tag{2.3}$$

provided $t \geq t_0 > 0$.

The idea of using the quantity $E(x,t)$ for obtaining heat kernel pointwise bounds is not new - it appeared in the works of Aronson [1] , [2] in the setting of parabolic equations in $\mathbf{R}^n$ and has been exploited in different contexts (see , for example, [9] , [57]) but we feel that the power of this tool has been underestimated as a direct way to connect the heat kernel and geometry.

Theorem 3 suggests the following universal approach for obtaining the off-diagonal pointwise upper bounds of the heat kernel - one might try first to estimate $E(x,t)$ as follows

$$E(x,t) \leq \frac{1}{f(t)} \tag{2.4}$$

which would imply immediately

$$p(x,y,t) \leq \frac{1}{f(t/2)} \exp\left(-\frac{r^2}{2Dt}\right) .$$

This method can be considered as an alternative to the well-known semigroup method of B.Davies [16] , [18] . The second ingredient of our approach is the way of obtaining (2.4) which is going to be discussed below in Section 3.

The estimate (2.2) and to some extent (2.3) are obtained in straightforward way from the semigroup property of the heat kernel upon a proper application of the Cauchy-Schwarz inequality. The other statements of the theorem are more subtle. Let us emphasize that for $D = 2$ the value of $E(x,t)$ may be equal to ∞ (as happens in $\mathbf{R}^n$) so that the hypothesis $D > 2$ is essential. Note also, that the monotone decrease of $E(x,t)$ is a consequence of the fact that the exponent $\xi(y,t) = \frac{r^2}{Dt}$ in the integral (2.1) satisfies the Hamilton-Jacobi inequality

$$\frac{\partial \xi}{\partial t} + \frac{1}{2} |\nabla \xi|^2 \leq 0 \tag{2.5}$$

which follows in turn from $|\nabla r| \leq 1$ and $D \geq 2$.

The inequality (2.5) makes a straightforward connection between the structure of the heat equation and geometry of the manifold via the distance function $r = \mathrm{dist}(x,y)$. The fact that the Gaussian exponent $\frac{r^2}{Dt}$ satisfies (2.5) is of great importance and this is why the Gaussian factor enters heat kernel estimations on arbitrary manifolds.

This phenomenon manifests itself in heat kernel estimates of other kinds, too. Technically, Aronson's approach based upon the Hamilton-Jacobi inequality works as follows. The heat equation is multiplied by the factor $\exp \xi(x,t)$ times the solution and, possibly, a cut-off function and integrated by parts. After suitable estimations by means of the Cauchy-Schwarz inequality a term appears containing the squared solution times the left-hand side of (2.5) which can be killed due to (2.5) . The power of this elementary trick is displayed by the fact that the following three theorems dealing with some integrals of the heat kernel can be proved by this method.

Theorem 4 *(Davies [22]) If A and B are two Borel subsets of M with finite volumes then*

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

where $d = \mathrm{dist}(A,B)$.

The term $-\lambda_1(M)t$ was absent in the Davies' original work. It was introduced in [32] where Theorem 4 was proved by means of the above method.

Theorem 5 *(Takeda [60] , Lyons [48]) Let A be a compact set with non-vanishing volume and let A^R denote the open R -neighbourhood of A where $R > 0$. Let $P(A,R)$ be the probability for the Brownian motion to exit A^R by a time $t > 0$ starting at a point of A provided the initial point is uniformly distributed in A, then*

$$P(R,T) \leq 16 \frac{\mathrm{Vol}\, A^R}{\mathrm{Vol}\, A} \int_R^\infty \frac{1}{(4\pi t)^{\frac{1}{2}}} \exp(-\frac{\eta^2}{4t}) d\eta \tag{2.6}$$

The inequality (2.6) implies the estimate of the heat kernel which is in some sense complementary to Theorem 4:

$$\int_A \int_{M \setminus A^R} p(x,y,t)dxdy \leq 16 \mathrm{Vol}\, A^R \int_R^\infty \frac{1}{(4\pi t)^{\frac{1}{2}}} \exp(-\frac{\eta^2}{4t}) d\eta .$$

Takeda's proof is purely probabilistic. As was demonstrated in [32] an inequality slightly different from (2.6) can be obtained again upon application of the technique based on Aronson's approach.

Theorem 6 *([26]) Let $v(r)$ be the volume of a geodesic ball of radius r with a fixed center on a geodesically complete Riemannian manifold M. If*

$$\int^{\infty} \frac{rdr}{\log v(r)} = \infty$$

then the manifold M is stochastically complete i.e. we have identically

$$\int_M p(x,y,t)dy = 1$$

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

This theorem was proved also by means of the same ideas as above. See [29] for a further development of this approach for an elliptic Schrödinger equation.

Theorems 4-6 are apart from our main direction and we have cited them only to illustrate the fact that Theorem 3 reflects the properties of the heat kernel deeply rooted in the nature of the heat equation.

The same method is applied to estimate derivatives of the heat kernel. Let us introduce the following quantities

$$E_m(x,t) = \int_M |\nabla^m p|^2 (x,y,t) \exp\left(\frac{r^2}{Dt} \right) dy$$

where $m \geq 0$ is an integer and ∇^m means $\Delta^{m/2}$ if m is even and $\nabla \Delta^{\frac{m-1}{2}}$ if m is odd (either operator Δ, ∇ relates to y). Let us note that $E_0(x,t)$ is exactly what we have denoted by $E(x,t)$.

Theorem 7 *([33]) If $D > 2$ then for any $x \in M$ the function $E_m(x,t)$ is a finite continuous decreasing function of t. Moreover, if $f(t)$ is a positive continuous function on $(0,T)$ where $0 < T \leq \infty$ and if for some $x \in M$ and for all $t \in (0,T)$ we have*

$$E(x,t) \leq \frac{1}{f(t)} \ ,$$

then for any $m \geq 1$ and for all $t \in (0,T)$

$$E_m(x,t) \leq \frac{\mathrm{const}_{m,D}}{f_m(t)} \tag{2.7}$$

f_m denotes the $m-$ th integral of f, namely,

$$f_0 = f, \quad f_m(t) = \int_0^t f_{m-1}(\tau)d\tau, \quad m \geq 1.$$

Obviously, the inequality (2.7) implies a universal estimate

$$E_m(x,t) \leq \frac{\mathrm{const}_{m,D}}{t^m} E(x, \frac{t}{2}) \ .$$

A similar estimate but without the Gaussian weight $\exp\left(\frac{r^2}{Dt} \right)$ was proved in [9] . The inequality (2.7) yields a sharper (and, apparently, the sharpest) dependence on t.

Pointwise estimates of the heat kernel time derivatives are obtained similar to Theorem 3.

Theorem 8 *([33]) For any two points $x, y \in M$ and for all $t > 0$*

$$\left| \frac{\partial^m p}{\partial t^m} \right| (x,y,t) \leq \sqrt{E_{2m}(x, \frac{t}{2}) E_0(y, \frac{t}{2})} \exp\left(-\frac{r^2}{2Dt} \right) \ .$$

where $m \geq 0$ is an integer and $r = \mathrm{dist}(x,y)$.

One could get also pointwise estimates of the gradient $\nabla_x p(x,y,t)$ in the same way if one knew a priori that two possible gradients $|\nabla_x p|$ and $|\nabla_y p|$ are equal or, at least finitely proportional which is generally false.

3. Pointwise Gaussian upper bounds

The task of this section is to show how to get an initial estimate (2.4) of $E(x,t)$ which would bring the theorems 3, 7, 8 to play. In contrast to these theorems which do not depend on geometry the inequality (2.4) must be derived from geometric assumptions. Fortunately, the Λ-isoperimetric inequality introduced in Section 1 works here as well.

The heart of the matter is the following mean-value type inequality.

Theorem 9 *([30] , [31]) Suppose that the Λ-isoperimetric inequality holds in a given geodesic ball $B_R^z \subset M$ of radius R centered at the point z. Let us consider along with the function $V(t)$ introduced by (1.8) also the function $W(r)$ defined as follows*

$$r = \int_0^{W(r)} \frac{dv}{v\sqrt{\Lambda(v)}} \tag{3.1}$$

(of course, we have to assume that this integral converges at 0).

Let $\mathcal{C}$ denote the cylinder $B_R^z \times (0,T)$, $T > 0$ and suppose that a function $u(x,t) \in C^\infty(\bar{\mathcal{C}})$ is a subsolution to the heat equation i.e. satisfies in $\mathcal{C}$ the inequality

$$u_t - \Delta u \leq 0 \ ,$$

then

$$u(z,T)_+^2 \leq \frac{\mathrm{const}}{\min\Big(TV(cT),\, R^2 W(cR)\Big)} \int_{\mathcal{C}} u_+^2 \tag{3.2}$$

where $c > 0$, const are absolute constants.

In the case of the Euclidean function $\Lambda(v) = \mathrm{const}\, v^{-2/n}$ we have $V(t) = \mathrm{const}\, t^{n/2}$ and $W(r) = \mathrm{const}\, r^n$. If we suppose in addition that $T = R^2$ which is the usual Euclidean scaling of the time and space variables then it follows that the factor in the front of the integral in (3.2) is proportional to $(\mathrm{Vol}\,\mathcal{C})^{-1}$, and we obtain the well-known mean value inequality of Moser [53] . This theorem is the only place where we make use of the Λ-isoperimetric inequality (except Theorem 1). All the subsequent results are obtained without appealing to geometry. Whenever Theorem 9 is improved - for example, we conjecture that the best value of the constant c therein is 1 - it will lead immediately to improvements in all the following heat kernel upper bounds.

In what follows, we always suppose that $\Lambda(v)$ is a given function on $(0,+\infty)$ such that the functions $V(t)$ and $W(r)$ defined by (1.8) and (3.1) do exist. Therefore, the functions $V(t)$ and $W(r)$ satisfy the conditions (i)-(iii) of Section 2. Moreover, we put a restriction on the function $V(t)$ which assumes some more regularity of this function and which is different from the regularity condition (iv) used in Theorem 2. Let us put $l(t) = t\frac{V'(t)}{V(t)}$ and suppose that

(v) for some $0 < T \leq \infty$ and $N > 0$

$$\begin{cases} l(t) \leq N \text{ if } t \leq 2T \\ l(t) \text{ is increasing if } t > T \end{cases} \tag{3.3}$$

This condition needs some comments. For all reasonable applications we have for small values of t that $V(t) = \mathrm{const} \cdot t^\nu$, $\nu > 0$. Therefore, for such t the function $l(t)$ is a constant. If this function remains bounded at ∞ then (3.3) is satisfied for $T = \infty$. Otherwise, the function $l(t)$ is unbounded and we may assume it to be monotonically increasing in a neighbourhood of ∞ (which corresponds to a finite value of T). Actually, the condition (v) prohibits jumps of the function $V(t)$.

Let us note also that the case $T = \infty$ takes place for a polynomial function $V(t)$ whereas a finite T occurs for a function $V(t)$ of a superpolynomial growth. At least the standard functions (1.21) satisfy (v).

Theorem 10 *([31]) Suppose that a Λ-isoperimetric inequality holds in the ball B_R^z and the function $V(t)$ satisfies the hypothesis (v). Let us introduce the function $\mathcal{R} = W^{-1} \circ V$ or, in other words,*

$$\mathcal{R}(t) = \int_0^{V(t)} \frac{dv}{v\sqrt{\Lambda(v)}}.$$

Then for all $t > 0$ such that

$$t \leq R^2, \ \ \mathcal{R}(ct) \leq cR \tag{3.4}$$

the estimate holds:

$$E(z,t) \leq \frac{\mathrm{const}_{D,N,T}}{V(\delta t)}$$

where $c>0$ is the absolute constant the same as in Theorem 9, $\delta = \delta(D)$ and $D>2$.

Thus, given a Λ-isoperimetric inequality in the ball B_R^z, we can estimate from above $E(z,t)$ for values of $t \leq t_0$ where t_0 is determined by (3.4) . This is not surprising from a probabilistic point of view: for small time a Brownian particle starting from the point z is found mainly inside the ball B_R^z, and the transition density $p(z,y,t)$ for $y \in B_R^z$ can be estimated in terms of intrinsic geometry of the ball as well as $E(z,t)$ because the points of this ball make the main contribution to the integral $E(z,t)$.

But for larger values of t geometry outside the ball plays a crucial role and one can not actually estimate the transition density when it really depends on unknown data. Nonetheless, it is still possible to say something about the quantity $E(x,t)$ simply due to its monotonicity: if $t>t_0$ then $E(z,t) \leq E(z,t_0)$. Therefore, we have, in fact, the upper bound of $E(z,t)$ for *all* values of time which makes Theorem 10 very flexible in applications.

Let us emphasize in this connection the role of the function $\mathcal{R}(t)$. One may conjecture that for the time t displacement of the Brownian particle does not exceed $\mathcal{R}(t)$ with a large probability. For example, for the Euclidean isoperimetric function $\Lambda(v) = \mathrm{const}\, v^{-2/n}$ we have $\mathcal{R}(t) = c_n\sqrt{t}$. For the function Λ defined by (1.15) (which is typical for a Cartan-Hadamard manifold of a strictly negative curvature) we have for large t that $\mathcal{R}(t) = \sqrt{\lambda}t + \mathrm{const}$. Finally, for the function (1.14) we get the function $\mathcal{R}(t)$ having an intermediate growth between $t^{\frac{1}{2}}$ and t for large t:

$$\mathcal{R}(t) \asymp t^{\frac{1+\alpha}{2+\alpha}}.$$

As soon as we are given a Λ-isoperimetric inequality on the manifold or in domains of the manifold then we can apply successively Theorems 10, 3, 8 in order to get pointwise upper bounds of the heat kernel and of its time derivatives. What follows are examples of application of this machinery.

Corollary 1 *([31]) Suppose that a Λ-isoperimetric inequality holds on the manifold M and the function $V(t)$ satisfies (v), then for all $x,y \in M,\ t>0$ and $D>2$ we have*

$$p(x,y,t) \leq \frac{\mathrm{const}}{V(\delta t)} \exp\left(-\frac{r^2}{2Dt}\right) \tag{3.5}$$

where $r = \mathrm{dist}(x,y),\ \delta = \delta(D) > 0$.

Let us compare this statement with Theorem 1: the corollary needs the additional hypothesis of regularity of $V(t)$ and yields a smaller coefficient δ than Theorem 1 but it introduces instead the Gaussian correction term into the upper bound.

A combination of the foregoing theorems yields the following

Corollary 2 *([31] , [33]) Let a function $V(t)$ satisfy all the hypotheses (ı)-(v) and suppose that for all $x \in M,\ t>0$*

$$p(x,x,t) \leq \frac{1}{V(t)}, \tag{3.6}$$

then the estimate (3.5) holds for all $x,y \in M$ and $t>0$. Moreover, for all $m = 1,2,...$ we have

$$\left|\frac{\partial^m p}{\partial t^m}\right|(x,y,t) \leq \frac{\mathrm{const}\ \exp\left(-\frac{r^2}{2Dt}\right)}{\sqrt{V(\delta t)V_{2m}(\delta t)}} \tag{3.7}$$

where V_k stands for the $k-$ th integral of $V(t)$ and $\delta = \delta(D) > 0$.

The proof can be seen from the diagram (all constant multiples are skipped here):

$$\begin{tikzcd}[column sep=small]
 & p \leq \frac{1}{V(t)} \arrow[d, "\text{theorem 2}"] & \\
 & \lambda_1(\Omega) \geq \Lambda(\operatorname{Vol}\Omega) \arrow[d, "\text{theorem 10}"] & \\
 & E(x,t) \leq \frac{1}{V(t)} \arrow[dl, "\text{theorem 3}"'] \arrow[dr, "\text{theorem 7}"] & \\
p \leq \frac{1}{V(t)} e^{-\frac{r^2}{2Dt}} & & E_m \leq \frac{1}{V_m(t)} \arrow[d, "\text{theorem 8}"] \\
 & & \left|\frac{\partial^m p}{\partial t^m}\right| \leq \frac{1}{\sqrt{V_{2m}V}} e^{-\frac{r^2}{2Dt}}
\end{tikzcd}$$

Results of the kind that (3.6) implies (3.5) were known before but only for a polynomial function $V(t)$. Apparently, for the first time such a statement was proved by Ushakov [61] for parabolic equations in unbounded domains of $\mathbf{R}^n$. His method goes through in our setting as well provided the function $V(t)$ grows at most polynomially in the sense that for all $t > 0$

$$V(2t) \leq \operatorname{const} V(t), \tag{3.8}$$

for example,

$$V(t) = \operatorname{const} \begin{cases} t^\gamma & , \ t \leq 1 \\ t^\mu & , \ t > 1 \end{cases} . \tag{3.9}$$

The advantage of Ushakov's proof is that it uses no isoperimetric properties - he deduced the Gaussian estimate (3.5) (albeit with a large D) directly from the on-diagonal upper bound (3.6) .

The theorem that (3.6) implies (3.5) provided $V(t)$ is the function (3.9) was first proved in the setting of Riemannian manifolds by Davies [16] using a log-Sobolev inequality as a bridge between (3.6) and (3.5) .

For a polynomial function $V(t)$ in the sense (3.8) one can simplify considerably either inequality (3.5) and (3.7) . Say, (3.7) becomes:

$$\left|\frac{\partial^m p}{\partial t^m}\right|(x,y,t) \leq \frac{\operatorname{const}}{t^m V(t)} \left(1 + \frac{r^2}{t}\right)^\nu \exp\left(-\frac{r^2}{4t}\right) \tag{3.10}$$

where $\nu = 1 + \frac{n}{2} + m$. The sharp factor $\frac{1}{4}$ in the Gaussian exponent appears when optimizing the initial estimate (3.7) containing the factor $\frac{1}{2D}$ with respect to $D > 2$ taking into account how the other coefficients are expressed through D. The polynomial correction term comes from this procedure and it can not be killed generally (see [50]). The sharpest form of this term is due to Davies and Pang [19] who showed that (3.6) for the function (3.9) implies the following

$$p(x,y,t) \leq \operatorname{const} \max\left(t^{-\gamma}(1 + \frac{r^2}{t})^\gamma, \ t^{-\mu}(1 + \frac{r}{t})^\mu\right) \exp\left(-\frac{r^2}{4t}\right) .$$

If the function $V(t)$ grows at least polynomially in the sense that for some $\kappa \in (0,1)$ and for all $t > 0$

$$\frac{VV''}{V'^2} \geq \kappa$$

(note, that (iii) implies $\frac{VV''}{V'^2} \leq 1$) then one can show that

$$\sqrt{VV_{2m}} \asymp V_m \asymp V\left(\frac{V}{V'}\right)^m$$

and (3.7) acquires the form

$$\left|\frac{\partial^m p}{\partial t^m}\right|(x,y,t) \le \frac{\text{const}}{V_m(\delta t)}\exp\left(-\frac{r^2}{2Dt}\right) \ .$$

As far as the time derivatives of the heat kernel are concerned, the sharpest result (again for the case of the function (3.9)) was due to Davies [21] (see also [66] for the setting of Lie groups). He proved a slightly sharper estimate than (3.10) with the exponent ν being 1 less than ours.

The Davies' method [21] is based heavily upon the analytic nature of the heat semigroup. This enables one to apply powerful tools of the theory of analytic functions but, on the other hand, it is not evident whether it works for a superpolynomial function $V(t)$, say, $V(t) = \exp(t^\alpha)$. A similar approach was used also by Varopoulos [64] , Kovalenko and Semenov [42] in other settings. Alternative methods of estimation of the time derivatives of the heat kernel can be found in works of Porper [56] (see also [57]) and Cheng, Li, Yau [9] .

Next we consider situations when a Λ-isoperimetric inequality is known in domains of the manifold rather than for the entire manifold.

Corollary 3 *([31] , [33]) On an arbitrary manifold M for all $x, y \in M$ and for all $t > 0$*

$$p(x,y,t) \le \frac{\Phi(x)\Phi(y)}{\min(t^{n/2},\ 1)}\left(1+\frac{r^2}{t}\right)^{1+\frac{n}{2}}\exp\left(-\frac{r^2}{4t}-\lambda t\right) \tag{3.11}$$

where λ is the spectral gap of the Laplacian and $\Phi(x)$ is a function which depends on the intrinsic geometry of the ball B_1^x and on λ.

Moreover, for any integer $m = 1, 2, ...$ we have

$$\left|\frac{\partial^m p}{\partial t^m}\right|(x,y,t) \le \frac{\text{const}\,\Phi(x)\Phi(y)}{t^m\min(t^{n/2},\ 1)}\left(1+\frac{r^2}{t}\right)^{\nu}\exp\left(-\frac{r^2}{4t}\right) \tag{3.12}$$

where $\nu = 1 + \frac{n}{2} + m$. If, in addition, $\lambda > 0$ then

$$\left|\frac{\partial^m p}{\partial t^m}\right|(x,y,t) \le \frac{\text{const}\,\Phi(x)\Phi(y)}{\min(t^{n/2+m},\ 1)}\left(1+\frac{r^2}{t}\right)^{\nu}\exp\left(-\frac{r^2}{4t}-\lambda t\right) \tag{3.13}$$

The reason why the manifold M may be arbitrary here is that for compactness arguments in any ball B_R^x a Λ-isoperimetric inequality holds with the function $\Lambda(v) = c_{x,R}v^{-2/n}$ similar to the Faber-Krahn inequality. The constant $c_{x,R} > 0$ depends, of course, upon geometry inside the ball and the function $\Phi(x)$ is expressed actually through $c_{x,1}$:

$$\Phi(x) = \text{const}_{n,\lambda}(c_{x,1})^{-n/4} \ .$$

For example, if all balls of the radius 1 have the same isoperimetric constant $c_{x,1}$ which occurs on manifolds of bounded geometry then (3.11) yields

$$p(x,y,t) \le \frac{\text{const}}{\min(t^{n/2},\ 1)}\left(1+\frac{r^2}{t}\right)^{1+\frac{n}{2}}\exp\left(-\frac{r^2}{4t}-\lambda t\right) \ . \tag{3.14}$$

Let us record also the fact that $\frac{\partial^m p}{\partial t^m}$ decays as $t \to \infty$ a priori at least as fast as t^{-m} which is seen from (3.12) . If $\lambda > 0$ then (3.13) provides the exponential decay $\exp(-\lambda t)$ as one might expect.

Corollary 4 *([31] , [33]) Suppose that the Λ-isoperimetric inequality holds in any ball $B_R^x \subset M$ with the following function $\Lambda = \Lambda_{x,R}$ depending on the ball in the following manner:*

$$\Lambda_{x,R}(v) = \frac{a}{R^2}\left(\frac{\operatorname{Vol}B_R^x}{v}\right)^{2/n},\ a > 0\ . \tag{3.15}$$

Then the we have the following heat kernel estimate for all $x, y \in M$ and $t > 0$

$$p(x,y,t) \le \frac{\text{const}}{\operatorname{Vol}B_{\sqrt{t}}^x}\left(1+\frac{r^2}{t}\right)^{1+\frac{3}{4}n}\exp\left(-\frac{r^2}{4t}\right) \tag{3.16}$$

as well as the estimate of the time derivatives:

$$\left|\frac{\partial^m p}{\partial t^m}\right|(x,y,t) \le \frac{\text{const}}{t^m \text{Vol}\, B^x_{\sqrt{t}}}\left(1+\frac{r^2}{t}\right)^{\nu}\exp\left(-\frac{r^2}{4t}\right)$$

where $\nu = 1 + \frac{3}{4}n + m,\ m = 1, 2, \dots$.

The hypothesis (3.15) looks at first sight somewhat exotic but actually it is very natural. In fact, it is equivalent to the combination of the following weaker version of (3.16)

$$p(x,x,t) \le \frac{\text{const}}{\text{Vol}\, B^x_{\sqrt{t}}}$$

and the following property of balls : for all $x \in M$ and $\rho < R$

$$\frac{\text{Vol}\, B^x_R}{\text{Vol}\, B^x_\rho} \le \text{const}\left(\frac{R}{\rho}\right)^n$$

(see Proposition 5.2 in [31]).

For example, (3.15) holds on a manifold of non-negative Ricci curvature. For the case of a non-negatively curved manifold, an estimate close to (3.16) was proved first by Li and Yau [45] . But in contrast to their result our statement is stable under a quasi-isometry and, thereby, provides the estimate (3.16) also for any Riemannian metric which is finitely proportional to a non-negatively curved one.

A similar estimate can be proved for manifolds with Ricci curvature bounded below by a constant $-K$ where $K > 0$. On such a manifold the Λ-isoperimetric inequality with the function (3.15) holds only in a ball of a bounded radius. Corollary 3 implies the following:

Corollary 5 *If the Ricci curvature of a manifold M is bounded below by a (negative) constant then for all $x, y \in M, t > 1$*

$$p(x,y,t) \le \frac{\text{const}}{\sqrt{\text{Vol}\, B^x_1 \text{Vol}\, B^y_1}}\left(1+\frac{r^2}{t}\right)^{1+\frac{n}{2}}\exp\left(-\frac{r^2}{4t} - \lambda t\right)$$

where $\lambda = \lambda_1(M)$.

See also [45] , [18] , [67] for the earlier results of this kind and [23] for the sharpest estimates.

The next statement is complementary to the preceding corollaries - it covers, in particular, simply connected manifolds of negative curvature i.e. Cartan-Hadamard manifolds. Let us fix some point $y \in M$ on an arbitrary manifold and let us denote by $\lambda(R)$ the spectral gap of the Laplacian in $L^2(M \setminus \overline{B^y_R})$. Evidently, $\lambda(R)$ is a non-negative increasing function of R. If, for example, M is a Cartan-Hadamard manifold then

$$\lambda(R) \ge \frac{1}{4}(n-1)^2 k(R)^2$$

provided $-k(R)^2$ is the supremum of the sectional curvature in the exterior of the ball B^y_R.

Corollary 6 *([31]) Suppose that a Λ-isoperimetric inequality holds on the whole manifold M with the Euclidean function*

$$\Lambda(v) = av^{-\frac{2}{n}},\ a > 0,$$

then for all $t > 0$ and for any $x \in M$ such that $r \equiv \text{dist}(x,y) > \sqrt{t}$ the inequality is valid

$$p(x,y,t) \le \frac{\text{const}}{t^{n/2}}\exp\left(-\delta\frac{r^2}{4t} - \delta\lambda(0)t - cr\sqrt{\lambda(\delta r)}\right) \tag{3.17}$$

where $\delta < 1$ is arbitrary and $c = c(\delta) > 0$.

The most interesting term here is the third factor $\exp\left(-cr\sqrt{\lambda(\delta r)}\right)$ which may decay as $r \to \infty$ faster than predicted by the Gaussian exponential provided the function $\lambda(r)$ grows fast enough.

A similar term is seen in the estimate (0.2) of the heat kernel on the hyperbolic space $\mathbf{H}^n_k$ - namely, this is $\exp(-\frac{n-1}{2}kr)$ while the third factor in (3.17) acquires in this case the form $\exp(-c\frac{n-1}{2}kr)$ which is essentially the same up to the constant factor c.

4. Harnack inequality

The classical Harnack inequality states that any positive harmonic function defined in a ball $B_R^z \subset \mathbf{R}^n$ satisfies the following inequality

$$\sup_{B_{R/2}^z} u \leq P \inf_{B_{R/2}^z} u \tag{4.1}$$

where $P = P(n)$. An analogous inequality holds for the heat equation in a cylinder $\mathcal{C} = B_R^z \times (0, R^2)$. Namely, if $u(x,t)$ is a positive solution in the cylinder $\mathcal{C}$, then

$$\sup_{\mathcal{C}_1} u \leq P \inf_{\mathcal{C}_2} u \tag{4.2}$$

where

$$\mathcal{C}_1 = B_{R/2}^z \times (\frac{1}{4}R^2, \frac{1}{2}R^2),\ \mathcal{C}_2 = B_{R/2}^z \times (\frac{3}{4}R^2, R^2)$$

and P again depends only on n .

The same inequalities hold for positive solutions of uniformly elliptic and parabolic equations in divergence form in $\mathbf{R}^n$ - these are the theorems of Moser [52] , [53] , [54] (see also [57]). In this case the constant P depends also on constants of ellipticity or parabolicity of the operator in question.

Obviously, the elliptic Harnack inequality follows from the parabolic one, so we shall treat here mainly the parabolic case which conforms also to the spirit of these notes.

By compactness arguments, Moser's theorems can be extended to arbitrary Riemannian manifold but in this setting the Harnack constant P in (4.2) (as well as in (4.1)) depends heavily on geometry inside the geodesic ball B_R^z. The major problem is to find sharp enough upper bounds of $P(B_R^z)$ but this problem is far from being solved.

In $\mathbf{R}^n$ the Harnack constant $P(B_R^z)$ is uniformly bounded from above, in $\mathbf{H}_k^n$ it behaves as $e^{CR},\ C > 0$ as $R \to \infty$. Let us consider also a manifold of Molchanov and Kuzmenko [43] which is constructed as follows: let us take two copies of $\mathbf{R}^n,\ n > 2$ cut off a unit ball from either space and glue their exteriors along the boundaries. For this manifold one can prove that $\sup_z P(B_R^z) \sim R^C,\ C > 0$ for a large R.

We are going to describe a class of manifolds where $P(B_R^z)$ remains uniformly bounded from above as in $\mathbf{R}^n$. The significance of such a uniform kind of the Harnack inequality is displayed by the following statement.

Proposition *Suppose that in any ball of a manifold M the parabolic Harnack inequality (4.2) holds with the same constant P. Then the heat kernel obeys the double-sided estimate*

$$\frac{\text{const}}{\operatorname{Vol} B_{\sqrt{t}}^x} \exp\left(-\frac{r^2}{2Ct}\right) \leq p(x,y,t) \leq \frac{\text{const}}{\operatorname{Vol} B_{\sqrt{t}}^x} \exp\left(-\frac{r^2}{2Dt}\right) \tag{4.3}$$

where $D > 2$ can be taken arbitrarily close to 2 and $C = C(P)$.

This is a kind of a statement whose proof has never been published explicitly although it is known very well for experts in this field. Whereas the deduction of the lower bound in (4.3) from the Harnack inequality goes back to Aronson [1] , [2] (see also [45] for the setting of manifolds where the factor $\operatorname{Vol} B_{\sqrt{t}}^x$ appeared explicitly) the upper bound is normally obtained by methods outlined in Section 3 without the Harnack inequality (which is reasonable because the upper bound needs fewer geometric assumptions than the Harnack inequality). Formally, the upper bound in (4.3) is derived upon subsequent application of the theorems 12 and 15 below and of Corollary 4.

The following theorem makes it clear which geometric properties are responsible for the parabolic Harnack inequality.

Theorem 11 *[30] , [59]) Suppose that a manifold M satisfies the following hypotheses*

(a) a doubling volume property: for any $x \in M$ and $R > 0$

$$\operatorname{Vol} B_R^x \leq A \operatorname{Vol} B_{R/2}^x$$

(b) a weak Poincaré inequality: for some constants $N > 1$ and $a > 0$, for any ball $B_R^x \subset M$ and for a function $f \in C^1(B_R^x)$

$$\int_{B_R^x} |\nabla f|^2 \geq \frac{a}{R^2} \inf_{\xi \in \mathbf{R}} \int_{B_{R/N}^x} (f - \xi)^2 . \tag{4.4}$$

Then the parabolic Harnack inequality (4.2) holds with the constant P depending only on A, a, N .

A geometric analysis of Moser's proofs [52] , [53] , [54] shows (see [3] , [71]) that his approach is based upon the following three geometric properties of $\mathbf{R}^n$ and it can be carried over to a manifold whenever the manifold satisfies them:

1° the doubling volume property (a);
2° the Poincaré inequality (b) in the strong form when $N = 1$;
3° the Sobolev inequality (1.2) .

The contribution of Theorem 11 is that the Sobolev inequality is excluded from this list and the Poincaré inequality is replaced by a weaker version. But most surprising is that a converse theorem does hold.

Theorem 12 *(Saloff-Coste [59]) Suppose that the Harnack inequality for the heat equation on a manifold M is known to be valid in any ball with the same constant P, then the doubling volume property (a) and the weak Poincaré inequality (b) hold with the constant A, a, N depending only on P.*

Theorem 11 was first proved in [30] as well as the part "Harnack inequality $\Longrightarrow$ (a)" of Theorem 12. Saloff-Coste [59] proved a more general version of Theorem 11 and Theorem 12 completely. Moreover, he proved a version of these theorems which states that the Harnack constant $P(B_R^x)$ remains uniformly bounded for all ball of the radius $R < \rho$ where ρ is a given positive number if and only if the doubling volume property (a) and Poincaré inequality (b) hold for all $R < \rho$.

Since the properties (a) and (b) are preserved by a quasi-isometric transformation of a manifold then we get the following consequence of the Theorems 11, 12.

Corollary 7 *(Saloff-Coste [59]) The uniform parabolic Harnack inequality is a quasi-isometry invariant.*

It is still unknown whether the elliptic Harnack inequality is stable under a quasi-isometry. At least the condition (a) is not necessary for the elliptic Harnack inequality. Indeed, as was remarked in [9] , for a $2-$ dimensional manifold M, the elliptic Harnack inequality follows from the upper bound of the volume:

$$\operatorname{Vol} B_R^x \le \operatorname{const} R^2 \tag{4.5}$$

supposed to be true for all $x \in M$ and all $R > 0$. It is easy to see that there exists a $2-$ dimensional manifold where (4.5) holds (thereby, the elliptic Harnack inequality holds too) but (a) does not.

The Theorems 11,12 give the complete description of manifolds with the uniform Harnack inequality in terms of the properties (a), (b). The next question is how to check whether they do hold (especially Poincaré inequality) on a given manifold. The following result is a sample of possible approaches to this question.

Suppose that any two distinct points $x, y \in M$ are connected by a curve $\gamma_{x,y} (= \gamma_{y,x})$ and let the family of all these curves satisfy the hypotheses:

1° any segment of any curve $\gamma_{x,y}$ belongs to the family too;
2° $\operatorname{length} \gamma_{x,y} \le C \operatorname{dist}(x, y)$

Let Γ_q^x be the homothety centered at the point $x \in M$ with the coefficient $q \in (0, 1)$ which maps a point $y \in M$ to a point $z \in \gamma_{x,y}$ such that $\operatorname{length} \gamma_{x,z} = q \operatorname{length} \gamma_{x,y}$.

Obviously, this is a straightforward extension of the notion of homothety in $\mathbf{R}^n$. Such a family of the curves $\gamma_{x,y}$ does exist on any complete manifold - for example, one takes $\gamma_{x,y}$ to be the shortest geodesic between x, y (if the shortest geodesic is not unique then one may take one of them arbitrarily).

Theorem 13 *([30]) Suppose that for any $q \in (\frac{1}{2}, 1)$, for any $x \in M$ and for any open bounded set $\Omega \subset M$ the image $\Omega_q \equiv \Gamma_q^x(\Omega)$ is measurable and*

$$\operatorname{Vol} \Omega_q \ge c \operatorname{Vol} \Omega$$

where $c > 0$ is the same for all x, q, Ω , then the conditions (a) and (b) hold with the constants A, a, N depending only on c, C .

As a consequence, the parabolic Harnack inequality is valid under the assumptions of Theorem 13 as well. It can be proved with ease that the hypotheses of Theorem 13 hold on a Riemannian manifold with a non-negative Ricci curvature provided $\gamma_{x,y}$ is the shortest geodesic between x, y.

For such manifolds the Harnack inequality was proved first by Yau [70] in the elliptic case and by Li and Yau [45] in the parabolic case in question. In fact, Li and Yau proved a pointwise estimate of derivatives of a positive solution which is based on a lower bound of the Ricci curvature and which implies the Harnack inequality upon integration along geodesics.

Theorem 14 *(Li-Yau [45]) If the Ricci curvature of a manifold is bounded below by a constant $-K$ (where $K \geq 0$) then for any positive solution $u(x,t)$ of the heat equation in $M \times (0,T)$ and for all $\alpha > 1,\ 0 < t < T$ we have*

$$\frac{|\nabla u|^2}{u^2} - \alpha \frac{u_t}{u} \leq \frac{n\alpha^2}{2t} + \frac{Kn\alpha^2}{4(\alpha-1)} .$$

This theorem has an additional benefit that it enables one to estimate the gradient of the heat kernel - see [21] for the best known results. Let us recall that in Section 3 we stated upper bounds for the time derivative of the heat kernel rather than that of the gradient although Theorem 7 does give the upper bound of the weighted integral of ∇p. The pont is that for pointwise estimations of ∇p one needs information about a modulus of continuity of the Riemannian tensor which can not be derived from the isoperimetric properties but follows from a condition on Ricci curvature.

Theorem 14 gives a sharp value of the Harnack constant in terms of curvature but, on the other hand, that means that the Harnack constant is expressed through the second derivatives of the Riemannian metric. In contrast to that, Theorem 11 provides a rough Harnack constant which, in return, depends only on the metric itself and does not involve any derivatives. Apparently, Theorem 11 can be carried over to non-smooth (Lipschitz) manifolds and to a uniformly parabolic equation with measurable coefficients.

In the rest of this Section, we shall discuss the ingredients of the proof of the main Theorem 11 following [30] .

PART 1. We meet here the Λ-isoperimetric inequality (3.15) again.

Theorem 15 *The hypotheses (a) and (b) imply that in any ball $B_R^x \subset M$ a Λ-isoperimetric inequality holds with the function*

$$\Lambda_{x,R}(v) = \frac{b}{R^2}\left(\frac{\operatorname{Vol} B_R^x}{v}\right)^{\beta} \tag{4.6}$$

where $b, \beta > 0$ are positive constants, depending on a, A, N.

Whenever we have known a Λ-isoperimetric inequality in a ball we can derive the mean-value type inequality of Theorem 9. In the situation of the Λ-isoperimetric inequality (4.6) it yields that for any subsolution u to the heat equation in the cylinder $\mathcal{C} = B_R^x \times (0, R^2]$, the following is true:

$$u(x,R^2)_+^2 \leq \frac{\text{const}}{\operatorname{Vol}\mathcal{C}} \int_{\mathcal{C}} u_+^2 \tag{4.7}$$

Let us recall that the first part of Moser's proof [53] is devoted exactly to obtaining the mean-value inequality (4.7) and this is the point where he used heavily the Sobolev inequality. Theorems 15 and 9 enabled us to avoid using the Sobolev inequality.

PART 2. Another distinction from Moser's setting is that we are given the weak Poincaré inequality (b) rather than the strong one. Actually, we do have the strong Poincaré inequality: as Jerison [38] showed the hypotheses (a) and (b) with $N > 1$ imply (b) with $N = 1$. The theorem of Jerison was applied by Saloff-Coste [59] in his alternative proof of Theorem 11 which follows mainly Moser's scheme.

In the original proof [30] , we did not use Jerison's theorem simply because Theorem 11 was discovered approximately at the same time as Jerison's (see the early announcement [27]). We first obtain a weak version of Harnack's inequality. Given a function $\delta(\varepsilon) : (0,1) \to (0,1)$, we say that a function v satisfies a *weak* Harnack inequality in a cylinder $\mathcal{C} = B_r^x \times (t, t+r^2)$ provided the following assertion is true:

If $v > 0$ in $\mathcal{C}$ and for some $0 < \varepsilon < 1$

$$\operatorname{Vol}\Big(\{v > 1\} \cap \mathcal{C}_1\Big) \geq \varepsilon \operatorname{Vol}\mathcal{C}_1$$

then

$$\inf_{\mathcal{C}_2} v \geq \delta(\varepsilon)$$

where

$$\mathcal{C}_1 = B_{r/2}^x \times (t, t + \frac{1}{4}r^2),\ \mathcal{C}_2 = B_{r/2}^x \times (t + \frac{3}{4}r^2, t + r^2) .$$

This kind of statement goes back to de Giorgi [24] and Moser [51] in the elliptic case and to Landis [44] in the parabolic one and has been normally applied in order to get Hölder continuity of solutions.

The following lemma is a point where the weak Poincaré inequality is used in a crucial manner. The mean-value inequality (4.7) is applied as well.

Lemma *If a manifold M satisfies the hypotheses (a) and (b) then any solution of the heat equation satisfies the weak Harnack inequality in any cylinder, whose height is equal to the squared radius, with the same function $\delta(\varepsilon)$ (in fact, δ depends on the constants A, a, N from (a) and (b), too).*

The next arguments are due to Landis who first found a straightforward (albeit a highly non-trivial) way to deduce the Harnack inequality from the weak one without applying again the heat equation.

Theorem 16 *(E.M.Landis) Let the doubling volume property (a) hold in the interior of a ball B_R^z (no Poincaré inequality is assumed to be true). Let a continuous positive function u be defined in a cylinder $\mathcal{C} = B_R^z \times (0, R^2)$ and suppose that for any function $v = C_1 u + C_2$ (where $C_{1,2}$ are arbitrary real numbers) in any sub-cylinder $B_r^x \times (t, t + r^2) \subset \mathcal{C}$ the weak Harnack inequality holds with the same function $\delta(\varepsilon)$. Then the normal Harnack inequality (4.2) is valid for the function u in $\mathcal{C}$, the Harnack constant P depending upon A and $\delta(\varepsilon)$.*

The method of the proof of this theorem in $\mathbf{R}^n$ appears in the survey by Kondratjev and Landis [41] although the main part of it was published much earlier - see [44] . It is a pleasure for me to thank Landis for his drawing my attention to this method.

The proof of Theorem 16 is reproduced in [30] in the context of manifolds (see the proof of Theorem 4.1 there) albeit without the explicit statement that u is not assumed to satisfy the heat equation.

In conclusion , we shall display graphically all dependences mentioned above:

$$\begin{tikzcd}
(a) \arrow[dr] \arrow[dddr] \arrow[ddddr] & & (b) \arrow[dl] \arrow[dddl] \\
& \Lambda - isoperimetric\ inequality \arrow[d] & \\
& mean - value\ inequality \arrow[d] & \\
& weak\ Harnack\ inequality \arrow[d] & \\
& Harnack\ inequality &
\end{tikzcd}$$

5. Manifolds with a local uniform structure

For an arbitrary manifold one can not expect any a priori decay of the heat kernel $p(x, y, t)$ as $t \to \infty$ unless the spectral gap of the Laplacian is known to be positive. Nonetheless, it turned out, that some local assumptions such as the hypothesis of bounded geometry, may lead to global non-trivial information concerning the heat kernel behaviour.

The starting point of our consideration is the conjecture of Varopoulos [62] , [65] that the heat kernel on a manifold of bounded geometry decays at least as fast as $t^{-\frac{1}{2}}$. He proved a weaker statement with the power $\frac{1}{2} - \varepsilon$ instead of $\frac{1}{2}$. The complete proof was published by Chavel and Feldman [8] and by Coulhon [13] . All these results were based upon the idea that a manifold of bounded geometry can be replaced by an appropriate graph and the heat diffusion - by a random walk on this graph (see also [34] , [47] , [39] , [40]). From this point of view, the rate of the heat kernel decay $1/\sqrt{t}$ is not unexpected because this is the magnitude of the heat kernel on the thinnest graph $\mathbf{Z}$.

We show here that our general approach to the heat kernel upper estimates via a Λ-isoperimetric inequality works in this situation as well and gives a direct proof of the result mentioned above.

Let us discuss the notion of bounded geometry which reflects the fact that a manifold is arranged similarly in a fixed size neighbourhood of any point. The standard definition is as follows.

Definition 3 The manifold M is said to have bounded geometry if the injectivity radius is uniformly bounded away from 0 and the Ricci curvature is uniformly bounded from below by a (negative) constant.

The drawback of this definition when dealing with heat kernel estimates is, first, that it restricts the topology of the manifold - any ball of the radius smaller than the injectivity radius must be homeomorphic to a Euclidean one; second, the assumption involving the curvature is not stable under quasi-isometry.

We introduce a more general concept which reflects the fact that balls of a given (small) size have similar intrinsic geometries and is very well suited for heat kernel estimation.

Definition 4 The manifold M is said to be *a locally Harnack manifold* if there is a positive radius $\rho > 0$ (which will be referred to as the Harnack radius) such that for any point $x \in M$ the following is true

(a) for any positive numbers $r < R < \rho$

$$\frac{\operatorname{Vol} B_R^x}{\operatorname{Vol} B_r^x} \le A\left(\frac{R}{r}\right)^n \tag{5.1}$$

(b) the weak Poincaré inequality (4.4) in any couple of concentric balls $B_{R/2}^x$, B_R^x provided $R < \rho$

If (a) were the doubling volume property from Section 4 then (a) and (b) would be exactly equivalent to the uniform parabolic Harnack inequality in any cylinder $B_R^x \times (0, R^2)$ where $R < \rho$. Of course, (a) implies the doubling volume property and, thereby, the Harnack inequality. Conversely, the doubling volume property implies (a) too, but with an exponent on the right-hand side of (5.1) which may differ from n.

The conditions (a) and (b) are valid, for example, whenever the manifold has Ricci curvature bounded below. On the other hand, this is still not enough to consider a manifold as being arranged locally uniformly - we shall consider along with (a) and (b) the additional condition:

(c) the volume of any ball B_ρ^x is uniformly bounded below by a positive constant v_0.

Theorem 17 *([28]) The hypotheses (a), (b), (c) imply that the manifold satisfies the Λ-isoperimetric inequality with the function*

$$\Lambda(v) = \frac{\text{const}}{\rho^2}\begin{cases} v^{-2/n} & , \ v \le v_0 \\ v^{-2} & , \ v > v_0 \end{cases}$$

where const *depends only on the constants involved in the conditions (a), (b).*

As a consequence of Theorem 17 and Corollary 1, we have the following statement.

Corollary 8 *For a locally Harnack manifold with the condition (c), the heat kernel satisfies the following estimate for all $x, y \in M$ and for all $t > \rho^2$*

$$p(x, y, t) \le \frac{\text{const}}{\sqrt{t}} \exp\left(-\frac{r^2}{2Dt}\right)$$

(where as usual $D > 2$) and the estimate of the time derivatives:

$$\left|\frac{\partial^m p}{\partial t^m}\right| (x, y, t) \le \frac{\text{const}}{t^{m+1/2}} \exp\left(-\frac{r^2}{2Dt}\right) \ , \ m = 1, 2, ...$$

Of course, it is possible to replace here D by 2 if one pays for it by the polynomial correction term as in Section 3.

As far as small values of time $t < \rho^2$ are concerned, the conditions (a), (b), (c) imply (similar to Theorem 15) that in any ball of the Harnack radius ρ, a Euclidean Λ-isoperimetric inequality holds which enables us to apply Corollary 3 and yields therefore the upper bound (3.14) .

It turns out that the condition (c) may be relaxed in the following way.

Theorem 18 *([28]) Suppose that M is a locally Harnack manifold and for a given point y the following holds:*

(c′) for any $x \in M$

$$\operatorname{Vol} B_\rho^x \ge v_0 r^{-\alpha}$$

where $r = \operatorname{dist}(x, y)$ and $v_0 > 0, \ 0 \le \alpha \le 1$.
Then for any $x \in M$ and $t > \rho^2$

$$\left|\frac{\partial^m p}{\partial t^m}\right| (x, y, t) \le \frac{\text{const}}{t^m \sqrt{t^{1-\alpha}}} \exp\left(-\frac{r^2}{2Dt}\right)$$

where $m = 0, 1, 2, ...$.

The last result to be presented here is a version of Theorem 1 when one knows the Λ-isoperimetric inequality only for large regions. The idea to consider isoperimetric properties only for regions containing a ball of a given radius was introduced by Chavel and Feldman [8] . They referred to it as a *modified* isoperimetric inequality. Of course, in order to operate with this inequality one should have known a priori information about small regions which is provided by a hypothesis of bounded geometry.

Theorem 19 *([28]) Let M be a locally Harnack manifold and x be a given (fixed) point on M. Suppose that for any pre-compact region Ω containing the ball B^x_ρ of the Harnack radius ρ, the following isoperimetric inequality holds*

$$\lambda_1(\Omega) \geq \Lambda(\mathrm{Vol}\,\Omega),$$

Λ being a positive continuous decreasing function defined on (v_0, ∞), where $v_0 = \mathrm{Vol}\, B^x_\rho$. Then for all $t > t_0 \equiv \delta\rho^2$ we have

$$p(x,x,t) \leq \frac{\mathrm{const}}{V(t/2)}$$

where the function $V(t)$ is defined from the relation

$$t - t_0 = \int_{v_0}^{V(t)} \frac{dv}{v\Lambda(v)}$$

and $\delta > 0$ depends on the constants from the conditions (a), (b).

If $t \leq t_0$ then

$$p(x,x,t) \leq \frac{\mathrm{const}}{t^{n/2}} \ .$$

Once we have due to this theorem the on-diagonal estimate of the heat kernel, we can run again the machinery of Sections 1-3 to obtain a Gaussian off-diagonal estimate and that of the derivatives.

REFERENCES

[1] **Aronson D.G.**, *Bounds for the fundamental solution of a parabolic equation*, Bull. of AMS, **73** (1967) pp. 890-896.

[2] **Aronson D.G.**, *Non-negative solutions of linear parabolic equations*, Ann. Scuola Norm. Sup. Pisa. Cl. Sci. (4), **22** (1968) pp. 607-694. Addendum **25** (1971) pp. 221-228.

[3] **Bombieri E., Giusti E.**, *Harnack's inequality for elliptic differential equations on minimal surfaces*, Invent. Math., **15** (1972) pp. 24-46.

[4] **Bougerol P.**, *Théorème central limite local sur certains groupes de Lie*, Ann. Sc. E.N.S. series 4, **14** (1981) pp. 403-432.

[5] **Carlen E.A., Kusuoka S., Stroock D.W.**, *Upper Bounds for symmetric Markov transition functions*, Ann. Inst. H. Poincaré, proba. et stat., suppl. au, no.2, (1987) pp. 245-287.

[6] **Carron G.**, *Inégalités isopérimétriques de Faber-Krahn et conséquences*, preprint.

[7] **Chavel I.**, "Eigenvalues in Riemannian geometry", Academic Press, New York, 1984.

[8] **Chavel I., Feldman E.**, *Modified isoperimetric constants, and large time heat diffusion in Riemannian manifolds*, Duke Math. J., **64** (1991) no.3, pp. 473-499.

[9] **Cheng S.Y., Li P., Yau S.-T.**, *On the upper estimate of the heat kernel of a complete Riemannian manifold*, Amer. J. Math., **103** (1981) no.5, pp. 1021-1063.

[10] **Coulhon T., Ledoux M.**, *Isoperimetrie, decroissance du noyau de la chaleur et transformations de Riesz: un conte-exemple*, preprint.

[11] **Coulhon T.**, *Inégalités de Gagliardo-Nirenberg pour les semi-groupes d'opérateurs et applications*, Potential Analysis, **1** (1992) pp. 343-353.

[12] **Coulhon T.**, *Sobolev inequalities on Graphs and manifolds*, in: Harmonic Analysis and Discrete Potential Theory, Plenum Press, New York and London, 1992.

[13] **Coulhon T.**, *Noyau de chaleur et discretisation d'une variété riemanniene*, Israel J. Math., **80** (1992) pp. 289-300.

[14] **Coulhon T., Saloff-Coste L.**, *Isopérimétrie pour les groupes et les variétés*, Revista Mathemática Iberoamericana, **9** no.2, (1993)

[15] **Davies B., Simon B.**, *Ultracontractivity and the heat kernel for Schrödinger operators and Dirichlet Laplacians*, J. Funct. Anal., **59** (1984) pp. 335-395.

[16] **Davies E.B.**, *Explicit constants for Gaussian upper bounds on heat kernels*, Amer. J. Math., **109** (1987) pp. 319-334.

[17] **Davies E.B., Mandouvalos N.**, *Heat kernel bounds on hyperbolic space and Kleinian groups*, Proc. London Math. Soc.(3), **52** (1988) no.1, pp. 182-208.

[18] **Davies E.B.**, *Gaussian upper bounds for the heat kernel of some second-order operators on Riemannian manifolds*, J. Funct. Anal., **80** (1988) pp. 16-32.

[19] **Davies E.B., Pang M.M.H.**, *Sharp heat kernel bounds for some Laplace operators*, Qurt. J. Math., **40** (1989) pp. 281-290.
[20] **Davies E.B.**, "Heat kernels and spectral theory", Cambridge: Cambridge University Press, 1989.
[21] **Davies E.B.**, *Pointwise bounds on the space and time derivatives of the heat kernel*, J. Operator Theory, **21** (1989) pp. 367-378.
[22] **Davies E.B.**, *Heat kernel bounds, conservation of probability and the Feller property*, J. d'Analyse Math., **58** (1992) pp. 99-119.
[23] **Davies E.B.**, *The state of art for heat kernel bounds on negatively curved manifolds*, Bull. London Math. Soc., **25** (1993) pp. 289-292.
[24] **de Giorgi E.**, *Sulla differenziabilita e l'analiticita delle estremali degli integrali multipli regolari*, Mem. Accad. Sci. Torino Cl. Sci. Fis. Mat. Nat., ser.3, **3** (1957) pp. 25-43.
[25] **Grigor'yan A.A.**, *Isoperimetric inequalities for Riemannian products*, (in Russian) Mat. Zametki, **38** (1985) no.4, pp. 617-626.
Engl. transl. Math. Notes, **38** (1985) pp. 849-854.
[26] **Grigor'yan A.A.**, *On stochastically complete manifolds*, (in Russian) DAN SSSR, **260** (1986) no.3, pp. 534-537.
Engl. transl. Soviet Math. Dokl., **34** (1987) no.2, pp. 310-313.
[27] **Grigor'yan A.A.**, *Isoperimetric inequalities on Riemannian manifolds and their applications to the Laplace and heat equations on manifolds*, (in Russian) in: USSR conference on geometry "in large", Novosibirsk, 1987. p.34.
[28] **Grigor'yan A.**, *Heat kernel on a manifold with a local Harnack inequality*, Comm. in Analysis and Geometry, **2** (1994) no.1, pp. 111-138.
[29] **Grigor'yan A.A.**, *Bounded solutions of the Schrödinger equation on non-compact Riemannian manifolds*, (in Russian) Trudy seminara I.G.Petrovskogo, (1989) no.14, pp. 66-77.
Engl. transl. Journal of Soviet Math., **51** (1990) no.3, pp. 2340-2349.
[30] **Grigor'yan A.A.**, *The heat equation on non-compact Riemannian manifolds*, (in Russian) Matem. Sbornik, **182** (1991) no.1, pp. 55-87.
Engl. transl. Math. USSR Sb., **72** (1992) no.1, pp. 47-77.
[31] **Grigor'yan A.**, *Heat kernel upper bounds on a complete non-compact manifold*, Revista Mathemática Iberoamericana, to appear.
[32] **Grigor'yan A.**, *Integral maximum principle and its applications*, Proc. of Edinburgh Royal Society, to appear.
[33] **Grigor'yan A.**, *Upper bounds of derivatives of the heat kernel on an arbitrary complete manifold*, J. Funct. Anal., to appear.
[34] **Gromov M.**, "Structures métriques pour les Variétés Riemannienes", Paris: Cedic/Ferdnand Nathan, 1981.
[35] **Gushchin A.K.**, *On the uniform stabilization of solutions of the second mixed problem for a parabolic equation*, (in Russian) Matem. Sbornik, **119(161)** (1982) no.4, pp. 451-508.
Engl. transl. Math. USSR Sb., **47** (1984) pp. 439-498.
[36] **Gushchin A.K., Michailov V.P., Michailov Ju.A.**, *On uniform stabilization of the solution of the second mixed problem for a second order parabolic equation*, (in Russian) Matem. Sbornik, **128(170)** (1985) no.2, pp. 147-168.
Engl. transl. Math. USSR Sb., **56** (1987) pp. 141-162.
[37] **Hoffman D., Spruck J.**, *Sobolev and isoperimetric inequalities for Riemannian submanifolds*, Comm. Pure Appl. Math., **27** (1974) pp. 715-725.
[38] **Jerison D.**, *The Poincaré inequality for vector fields satisfying Hörmander condition*, Duke Math. J., **53** (1986) pp. 503-523.
[39] **Kanai M.**, *Rough isometries, and combinatorial approximations of geometries of noncompact Riemannian manifolds*, J. Math. Soc. Japan, **37** (1985) pp. 391-413.
[40] **Kanai M.**, *Rough isometries and the parabolicity of manifolds*, J. Math. Soc. Japan, **38** (1986) pp. 227-238.
[41] **Kondratjev V.A., Landis E.M.**, *A qualitative theory of second-order linear partial differential equations*, (in Russian) in: Itogi Nauki i Techniki, serija Sovremennye Problemy Matematiki, Fundamental'nye Napravlenija, **32** VINITI, Moscow, 1988. pp. 99-215.
[42] **Kovalenko V.P., Semenov U.A.**, *Semigroups generated by an elliptic operator of second order*, (in Russian) in: Methods of Functional Analysis in Problems of Mathematical Physics, Kiev Inst. of Math., Ukranian Acad. of Sciences, 1987. pp. 17-36.

[43] **Kuzmenko Yu.T., Molchanov S.A.**, *Counter-examples for Liouville-type theorems*, (in Russian) Vestnik MGU, ser. 1 Matematika, (1979) no.6, pp. 39-43.

[44] **Landis E.M.**, "The second order equations of elliptic and parabolic type", (in Russian) Nauka, Moscow, 1971.

[45] **Li P., Yau S.-T**, *On the parabolic kernel of the Schrödinger operator*, Acta Math., **156** (1986) no.3-4, pp. 153-201.

[46] **Lunt J.B.**, *Measurable Perturbations of Diffusions on Manifolds*, Thesis, University of Edinburgh, 1992.

[47] **Lyons T., Sullivan D.**, *Function theory, random paths and covering spaces*, J. Diff. Geom., **19** (1984) pp. 299-323.

[48] **Lyons T.**, *Random thoughts on reversible potential theory*, in: Summer School in Potential Theory, Joensuu 1990, edited by Ilpo Laine, University of Joensuu. Publications in Sciences 26, ISBN 951-696-837-6., pp. 71-114.

[49] **Maz'ya V.G.**, "Sobolev spaces", (in Russian) Izdat. Leningrad Gos. Univ. Leningrad, 1985.
Engl. transl. Springer-Verlag, 1985.

[50] **Molchanov S.A.**, *Diffusion processes and Riemannian geometry*, Russian Math. Surveys, **30** (1975) no.1, pp. 1-63.

[51] **Moser J.**, *A new proof of de Giorgi's theorem concerning the regularity problem for elliptic differential equations*, Comm. Pure Appl. Math., **13** (1960) pp. 457-468.

[52] **Moser J.**, *On Harnack's theorem for elliptic differential equations*, Comm. Pure Appl. Math., **14** (1961) pp. 577-591.

[53] **Moser J.**, *A Harnack inequality for parabolic differential equations*, Comm. Pure Appl. Math., **17** (1964) pp. 101-134.

[54] **Moser J.**, *On a pointwise estimate for parabolic differential equations*, Comm. Pure Appl. Math., **24** (1971) pp. 727-740.

[55] **Nash J.**, *Continuity of solutions of parabolic and elliptic equations*, Amer. Math. J., **80** (1958) pp. 931-954.

[56] **Porper F.O.**, *Estimates of the derivatives of the fundamental solution of a stationary parabolic divergence equation with constants that do not depend on the smoothness of the coefficients*, (in Russian) Dokl. AN SSSR, **235** (1977) pp. 1022-1025.
Engl. transl. Soviet Math. Dokl., **18** (1977) pp. 1092-1096.

[57] **Porper F.O., Eidel'man S.D.**, *Two-side estimates of fundamental solutions of second-order parabolic equations and some applications*, (in Russian) Uspechi Mat. Nauk, **39** (1984) no.3, pp. 101-156.
Engl. transl. Russian Math. Surveys, **39** (1984) no.3, pp. 119-178.

[58] **Robinson D.W.**, "Elliptic operators and Lie groups", Oxford New York Tokyo, Clarenton Press, Oxford Math. Mono., 1991.

[59] **Saloff-Coste L.**, *A note on Poincaré, Sobolev and Harnack inequality*, Duke J. Math, **65** no.3, (1992) pp. 27-38.

[60] **Takeda M.**, *On a martingale method for symmetric diffusion process and it's applications*, Osaka J. Math, **26** (1989) pp. 605-623.

[61] **Ushakov V.I.**, *Stabilization of solutions of the third mixed problem for a second order parabolic equation in a non-cylindric domain*, (in Russian) Matem. Sbornik, **111** (1980) pp. 95-115.
Engl. transl. Math. USSR Sb., **39** (1981) pp. 87-105.

[62] **Varopoulos N.Th.**, *Brownian motion and random walks on manifolds*, Ann. Inst. Fourier (Grenoble), **34** (1984) pp. 243-269.

[63] **Varopoulos N.Th.**, *Hardy-Littlewood theory for semigoups*, J. Funct. Anal., **63** (1985) no.2, pp. 240-260.

[64] **Varopoulos N.Th.**, *Semi-groupes d'opérateurs sur les espaces L^p*, C. R. Acad. Sci. Paris Sér. I Math., **301** (1985) pp. 865-868.

[65] **Varopoulos N.Th.**, *Random walks and Brownian motion on manifolds*, Sympos. Math., **29** (1986) pp. 97-109.

[66] **Varopoulos N.Th.**, *Analysis on Lie groups*, J. Funct. Anal., **76** (1988) pp. 346-410.

[67] **Varopoulos N.Th.**, *Small time Gaussian estimates of heat diffusion kernel.I. The semigroup technique*, Bull. Sci. Math.(2), **113** (1989) no.3, pp. 253-277.

[68] **Varopoulos N.Th.**, *Groups of superpolynomial growth*, in: Proceedings of the ICM satellite conference on Harmonic analysis, Springer, 1991.

[69] **Varopoulos N.Th., Saloff-Coste L., Coulhon T.**, "Analysis and geometry on groups", Cambridge University Press, Cambridge U.K., 1992.

[70] **Yau S.-T.**, *Harmonic functions on complete Riemannian manifolds*, Comm. Pure Appl. Math., **28** (1975) pp. 201-228.

[71] **Yau S.-T.**, *Survey on partial differential equations in differential geometry*, Ann. Math. Studies, **102** (1982) pp. 3-70.