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GAUSSIAN UPPER BOUNDS FOR THE HEAT KERNEL ON ARBITRARY MANIFOLDS

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1. Introduction

In this paper, we develop a universal way of obtaining Gaussian upper bounds of the heat kernel on Riemannian manifolds. By the word "Gaussian" we mean those estimates which contain a Gaussian exponential factor similar to one which enters the explicit formula for the heat kernel of the conventional Laplace operator in $\mathbb{R}^n$:

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

The history of the heat kernel Gaussian estimates started with the works of Nash [25] and Aronson [2] where the double-sided Gaussian estimates were obtained for the heat kernel of a uniformly parabolic equation in $\mathbb{R}^n$ in a divergence form (see also [15] for the improvement of the original Nash's argument and [26] for a consistent account of the Aronson's results and related topics). In particular, the Aronson's upper bound for the case of time-independent coefficients which is of interest for us reads as follows:

$$p(x,y,t)\le\frac{\mathrm{const}}{t^{n/2}}\exp\left(-\frac{|x-y|^2}{Ct}\right),$$

where C is a large enough constant.

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In a series of works of Gushin [22], [21] he extended the Gaussian upper bounds to parabolic equations in unbounded domains in $\mathbb{R}^n$ with the Neumann boundary condition.

As far as Riemannian manifolds are concerned, the heat kernel Gaussian upper bound first appeared in the work of Cheng, Li and Yau [7] for the case of complete manifolds of a bounded sectional curvature, and was extended soon by a different method in [6] to manifolds with bounded geometry. The most advanced and sharp results under the curvature assumptions were obtained by Li and Yau [24] by using their famous gradient estimates.

Given a Riemannian manifold M, one considers the associated Laplace operator Δ, its (minimal) heat kernel $p(x,y,t)$, and expects to have a Gaussian upper bound as follows

$$p(x,y,t) \le \frac{\mathrm{const}}{f(t)} \exp\left(-\frac{r^2}{Ct}\right), \tag{1.1}$$

where $r = \mathrm{dist}(x,y)$ is a geodesic distance between x, y, and $f(t)$ is some increasing function. In the works, cited above, such estimate was shown to be true on certain manifolds subject to curvature restrictions, with the constant C arbitrarily close to the ideal value 4.

The next crucial step was done by B. Davies who developed in a series of his works [11], [12], [9], [10] a powerful abstract method which enabled him to deduce the heat kernel Gaussian upper bounds from the log-Sobolev inequality. This method is robust in contrast to those based on Riemannian curvature. For example, it is invariant under a quasi-isometric transformation of the metric.

An alternative robust method based on a Faber-Krahn type inequalities was introduced by the author in [18] (see also [19], [20]). In particular, it was shown in [18] that *any* complete manifolds admits the estimate

$$p(x,y,t) \le \varphi(x,t)\varphi(y,t) \exp\left(-\frac{r^2}{Ct}\right)$$

(where the function $\varphi(x,t)$ is expressed in geometric terms) which suggests that the Gaussian exponential factor has a non-geometric nature.

The common achievement of the cited above works is understanding that the Gaussian upper bound (1.1) is virtually equivalent to a (logically) weaker on-diagonal bound

$$p(x,y,t) \le \frac{\mathrm{const}}{f(t)}, \tag{1.2}$$

which does not take into account the distance between x, y. Indeed, first let $f(t) = t^{n/2}$, where $n = \dim M$. Then the fact that (1.2) is true for all $x, y \in M$, and for all $t > 0$ is equivalent to each of the following functional inequalities:

1° a proper Sobolev inequality as proved by Varopoulos [28];

2° a Nash type inequality by Carlen, Kusuoka, Stroock [3];

3° a log-Sobolev inequality by Davies [11];

4° a Faber-Krahn type inequality by [18] and by Carron [4].

On the other hand, each of these functional inequalities implies also the Gaussian upper bound (1.1) with the same function $f(t)$. See [5] for a more geometric approach based on modified isoperimetric constants. See [23], [13] for the setting of graphs, [8], [29], [30] for Lie groups, and [1] for symmetric spaces.

The fact that an on-diagonal upper bound implies a Gaussian one was extended to more general class of functions $f(t)$ (including those of superpolynomial growth) by Davies [10] and by the author [18], again by using a bridging functional inequality.

At the same time, there is a direct way of deducing a Gaussian upper bound from an on-diagonal one which appeared first in the work of Ushakov [27] for the case of a polynomial function $f(t)$ and for the parabolic equation in the Euclidean space. This method was adapted later for manifolds in [16] but still within a polynomial setting.

The main purpose of the present paper is to extend this method to a wider class of the functions $f(t)$ including sub- and superpolynomially growing functions. The main result is the following theorem.

Theorem 1.1. *Let x, y be two points on an arbitrary smooth connected Riemannian manifold M, and let us have for all $t \in (0, T)$ (where T may be equal to ∞ or be a positive number)*

$$p(x, x, t) \leq \frac{1}{f(t)} \tag{1.3}$$

and

$$p(y, y, t) \leq \frac{1}{g(t)}, \tag{1.4}$$

*where f, g are functions regular in some sense (*see Section 2 below for the definition*). Then for any $C > 4$, for some $\delta = \delta(C) > 0$, and all $t \in (0, T)$,*

$$p(x, y, t) \leq \frac{\text{const}}{\sqrt{f(\delta t) g(\delta t)}} \exp\left(-\frac{r^2}{Ct}\right), \tag{1.5}$$

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

Let us emphasize the fact that unlike the functional-theoretic methods cited above, this theorem assumes the on-diagonal upper bounds only at *two* points x, y rather than at any point. The regularity condition is wide enough to include such functions as $\log^a t$, t^b, $\exp t^c$ and their combinations.

Needless to say that Theorem 1.1 recovers all Gaussian upper bounds obtained previously, and provides a simple way to produce such bounds automatically whenever one has proved a (much simpler) on-diagonal estimate.

2. Integral estimates of solutions

Let M denote any smooth connected Riemannian manifold (not necessarily complete), and let Ω be a pre-compact region on M with a smooth boundary. We allow M to have a boundary. If this is the case, then part of the boundary of Ω may be located on ∂M. In fact, $\overline{\Omega}$ will be treated as a compact manifold with a boundary.

We consider a function $u(x, t)$ defined on $\overline{\Omega} \times (0, +\infty)$ which is smooth enough and satisfies the following conditions:

$$\begin{cases} u(u_t - \Delta u) \leq 0, \\ u\frac{\partial u}{\partial \nu}\big|_{x \in \partial\Omega, t > 0} \leq 0, \\ u\big|_{x \notin K, t=0} = 0, \end{cases} \tag{2.1}$$

where ν is the outward normal vector field on the boundary $\partial\Omega$, K is a compact in Ω (the initial condition is understood in the sense that $u(x, t) \to 0$ as $t \to 0+$ locally uniformly in $x \in \Omega \setminus K$).

For example, u may be a solution to the Dirichlet or Neumann problem for the heat equation in $\Omega \times (0, +\infty)$ (with an initial condition having a support on K) or a positive subsolution, or a negative supersolution.

We will consider two integrals of u :

$$I(t)=\int_{\Omega}u^{2}(x,t)dx,$$
$$E_{D}(t)=\int_{\Omega}u^{2}(x,t)\exp\left(\frac{\operatorname{dist}^{2}(x,K)}{Dt}\right)dx,$$

where D is a positive number. Of course, we have always

$$I(t)\leq E_{D}(t).$$

The main result to be proved here is that to some extend there is a reverse inequality. But before we are able to state that, we have to introduce a technical regularity hypothesis on a function of a single variable.

Definition. We say that a function $f(t)$ defined for $t\in(0,\infty)$ is *regular* if:

1° it is positive;

2° it is monotonically increasing;

3° there are numbers $A\geq 1$ and $\gamma>1$ such that for all $0<t_1<t_2$ the following inequality holds:

$$\frac{f(\gamma t_1)}{f(t_1)}\leq A\frac{f(\gamma t_2)}{f(t_2)}. \tag{2.2}$$

Examples. 1. Let the function $f(t)$ be of *at most polynomial* growth in the sense that for all $t>0$ and some $\gamma>1$,

$$f(\gamma t)\leq Af(t). \tag{2.3}$$

Then (2.2) is obviously true. Indeed, we have

$$\frac{f(\gamma t_1)}{f(t_1)}\leq A\leq A\frac{f(\gamma t_2)}{f(t_2)}, \tag{2.4}$$

because $f(\gamma t_2)\geq f(t_2)$. Examples of the functions satisfying (2.3) are: $f(t)=t^{n}$, $f(t)=\log^{n}(1+t)$ (where $n>0$) etc.

2. Let $f(t)$ be of *at least polynomial* growth in the sense that for some $\gamma>1$ the quotient

$$\frac{f(\gamma t)}{f(t)} \tag{2.5}$$

is increasing in t. Then (2.2) holds again at this time with $A = 1$ because by monotonicity of (2.5)

$$\frac{f(\gamma t_1)}{f(t_1)} \leq \frac{f(\gamma t_2)}{f(t_2)}. \tag{2.6}$$

Examples of such functions are: $f(t) = t^n$, $f(t) = e^{t^n}$ etc.

3. Let us combine the two situations above: suppose that there is some $T > 0$ such that for all $t < T$ the inequality (2.3) holds while for $t > T$ the ratio (2.5) is increasing. Then $f(t)$ is regular again. Indeed, in order to check (2.2), let us consider two cases: $t_1 < T$ and $t_1 \geq T$. In the first case, we have again (2.4), while in the second case we repeat (2.6).

An example of a function which fits this case is:

$$f(t) = \begin{cases} c_1 t^n, & t < T, \\ c_2 e^{t^m}, & t \geq T, \end{cases}$$

where $n > 0, m > 0$, and the constants $c_{1,2}$ are chosen to ensure continuity (and, therefore, also monotonicity) of $f(t)$.

Now we can state our main technical result.

Theorem 2.1. *Let us suppose that $u(x,t)$ satisfies (2.1), and for any $t > 0$ we have*

$$I(t) \leq \frac{1}{f(t)}, \tag{2.7}$$

where the function $f(t)$ is regular as above. Then for any $D > 2$ and all $t > 0$

$$E_D(t) \leq \frac{4A}{f(\delta t)},$$

where $\delta = \delta(D, \gamma) > 0$.

Proof of the theorem. The proof will consist of three steps. In the first step, we will estimate the integral

$$I_R(t) = \int_{\Omega \setminus K^R} u^2(x,t)dx,$$

where K^R is the open $R-$neighbourhood of the set K. In the second step, we will estimate $E_D(t)$ for large D applying the upper bounds for $I_R(t)$, and, finally, in the third step, we will finish the proof for all $D > 2$.

STEP 1. Let us prove the following key lemma. The statement of this kind seems to have appeared for the first time in the paper of Ushakov [27] for the case of a polynomial function $f(t)$ and in the Euclidean space. We modified his approach and made it work for a more general function $f(t)$.

Lemma 2.2. *Under the hypotheses of Theorem 2.1, there exists $D_0 = D_0(\gamma) > 2$ such that*

$$I_R(t) \leq \frac{2A}{f(t/\gamma)} \exp\left(-\frac{R^2}{D_0 t}\right)$$

for all $R > 0$ and $t > 0$, where the constants A, γ are those from the regularity hypothesis (2.2).

Proof of Lemma 2.2. The idea of the proof is to compare the quantities $I_R(t)$ and $I_\rho(\tau)$ for $\rho < R$, $\tau < t$ in the following way:

$$I_R(t) \leq I_\rho(\tau) + \frac{1}{f(\tau)} \exp\left(-\frac{(R-\rho)^2}{2(t-\tau)}\right). \tag{2.8}$$

After we have shown (2.8),we will arrange sequences $\{R_k\}, \{t_k\}$ (where $k = 0, 1, 2, ...$) which start with R and t respectively and are decreasing so that $R_k \to R/2$ and $t_k \to 0$ as $k \to \infty$. Applying (2.8) to the consecutive pairs (R_k, t_k) and (R_{k+1}, t_{k+1}) and summing up all those inequalities, we obtain an upper bound for $I_R(t)$ in terms of a series which can be dealt with by taking specific sequences R_k, t_k.

We will finish this argument later but first we turn to the proof of (2.8). We apply the integral maximum principle, which states the following.

Proposition 2.3. *If $u(x,t)$ is smooth enough in $\overline{\Omega} \times (0,T)$ and satisfies the conditions*

$$\begin{cases} u(u_t - \Delta u) \leq 0, \\ u\frac{\partial u}{\partial \nu}\Big|_{x\in\partial\Omega, t\in(0,T)} \leq 0, \end{cases} \tag{2.9}$$

then the integral

$$\int_\Omega u^2(x,t) e^{\xi(x,t)} dx \tag{2.10}$$

is a decreasing function of $t \in (0,T)$ provided the function $\xi(x,t)$ is Lipschitz in $\overline{\Omega} \times (0,T)$ and satisfies the inequality

$$\xi_t + \frac{1}{2}|\nabla \xi|^2 \le 0. \tag{2.11}$$

This property of solutions to the heat equation is well known and goes back to the famous Aronson's paper [2]. Thereafter, it was proved for different settings in various works; see, for example, [7], [26], [19]. The actual proof is very simple and consists of taking the time derivative of the integral (2.10) and of applying integration by parts:

$$\begin{aligned}
\frac{d}{dt}\int_\Omega u^2 e^\xi &= \int_\Omega \xi_t u^2 e^\xi + \int_\Omega 2uu_t e^\xi \\
&\le \int_\Omega \xi_t u^2 e^\xi + \int_\Omega 2u\Delta u e^\xi \\
&\le \int_\Omega \xi_t u^2 e^\xi + \int_{\partial\Omega} 2u\frac{\partial u}{\partial \nu} e^\xi - 2\int_\Omega (\nabla(ue^\xi), \nabla u) \\
&\le -\frac{1}{2}\int_\Omega |\nabla \xi|^2 u^2 e^\xi - 2\int_\Omega u(\nabla\xi, \nabla u)e^\xi - 2\int_\Omega |\nabla u|^2 e^\xi \\
&= -\frac{1}{2}\int_\Omega (u\nabla\xi + 2\nabla u)^2 e^\xi \le 0.
\end{aligned}$$

q.e.d.

Let us note that we have used here at full strength the hypotheses (2.9) and (2.11) on the functions u and ξ respectively. Moreover, this is the only place where we need (2.9) and (2.11). In the proof of Theorem 2.1 which follows, we will apply the two first conditions from (2.1) ("the equation" and "the boundary condition") only via Proposition 2.3. On the contrary, we will use the initial condition of (2.1) explicitly.

We will be applying (2.11) with different functions ξ. Let us note that any function of the form

$$\xi(x,t) = \frac{d(x)}{D(t-s)}$$

fits (2.11) provided $d(x)$ is a distance function to some subset of M, $D \ge 2$, and the point s does not belong to $(0,T)$ (to ensure no singularities).

In order to prove (2.8), we choose some s, T such that $s > T > t$, and put $d(x)$ to be the distance to the exterior of the set K^R, i.e.,

$$d(x) = \begin{cases} R - \operatorname{dist}(x,K), & x \in K^R, \\ 0, & x \notin K^R. \end{cases}$$

By the integral maximum principle, we have

$$\int_\Omega u^2(x,t)\exp\left(-\frac{d(x)^2}{2(s-t)}\right) \le \int_\Omega u^2(x,\tau)\exp\left(-\frac{d(x)^2}{2(s-\tau)}\right).$$

Now we replace the left-hand side integral by a less value $I_R(t)$ because $d(x)$ vanishes off the set K^R. Then, we split the right-hand side integral into two parts: over the interior of K^ρ and over its exterior. In the first part, the exponential weight is bounded from above by

$$\exp\left(-\frac{(R-\rho)^2}{2(s-\tau)}\right),$$

since the distance from any point of K^ρ to the exterior of K^R is at least $R-\rho$. In the second part, we replace the exponential weight simply by the larger 1, obtaining, thus, $I_\rho(\tau)$. Therefore, we have

$$I_R(t) \le \exp\left(-\frac{(R-\rho)^2}{2(s-\tau)}\right)\int_{K^\rho} u^2(x,\tau)dx + I_\rho(\tau).$$

Finally, we apply the hypothesis (2.7) in the form

$$\int_{K^\rho} u^2(x,\tau)dx \le \frac{1}{f(\tau)},$$

and let $s \to t+$ whence (2.8) follows.

Given R and t, we consider the sequences $\{R_k\}$ and $\{t_k\}$, $k = 0, 1, 2, ...$ such that:

1° $\{R_k\}$ and $\{t_k\}$ are decreasing in k;

2° $R_0 = R$ and $R_k \to \frac{1}{2}R$ as $k \to \infty$;

3° $t_0 = t$ and $t_k \to 0$ as $k \to \infty$.

Applying (2.8) for the consecutive pairs (R_k, t_k) and (R_{k+1}, t_{k+1}) we obtain

$$\begin{aligned} I_{R_k}(t_k) \le\ & I_{R_{k+1}}(t_{k+1}) \\ & + \frac{1}{f(t_{k+1})}\exp\left(-\frac{(R_k - R_{k+1})^2}{2(t_k - t_{k+1})}\right). \end{aligned} \tag{2.12}$$

Let us note that $I_{R_k}(t_k) \to 0$ as $k \to \infty$. Indeed,

$$\lim_{k\to\infty} I_{R_k}(t_k) = \int_{\Omega\setminus K^{\frac{1}{2}R}} u^2(x,0)dx = 0,$$

because of the initial condition (2.1) for the function u.

Hence, we can sum up the inequalities (2.12) over all $k = 0, 1, 2, ...$ and obtain

$$I_R(t) \le \sum_{k=0}^{\infty} \frac{1}{f(t_{k+1})} \exp\left(-\frac{(R_k - R_{k+1})^2}{2(t_k - t_{k+1})} \right). \tag{2.13}$$

Let us specify the sequences R_k, t_k in the following way: we take

$$R_k = (\frac{1}{2} + \frac{1}{k+2})R$$

and

$$t_k = t/\gamma^k.$$

Since

$$R_k - R_{k+1} \ge \frac{R}{(k+3)^2}$$

and

$$t_k - t_{k+1} = \frac{(\gamma - 1)t}{\gamma^{k+1}},$$

we can expand (2.13) as follows

$$I_R(t) \le \sum_{k=0}^{\infty} \frac{1}{f(t_{k+1})} \exp\left(-\frac{\gamma^{k+1}}{(k+3)^4(\gamma - 1)} \frac{R^2}{2t} \right).$$

Let us estimate $f(t_{k+1})$ as follows. According to the property of the function $f(\cdot)$ to be regular, we have the following sequence of inequalities:

$$\frac{f(t_k)}{f(t_{k+1})} \le A \frac{f(t_0)}{f(t_1)},$$
$$\frac{f(t_{k-1})}{f(t_k)} \le A \frac{f(t_0)}{f(t_1)},$$
$$...$$
$$\frac{f(t_0)}{f(t_1)} \le A \frac{f(t_0)}{f(t_1)}.$$

Multiplying all them we derive

$$\frac{f(t_0)}{f(t_{k+1})} \le \left(A \frac{f(t_0)}{f(t_1)} \right)^{k+1},$$

whence we get

$$I_R(t) \leq \frac{1}{f(t)} \sum_{k=0}^{\infty} \exp\left((k+1) \log A \frac{f(t_0)}{f(t_1)} - \frac{\gamma^{k+1}}{(k+3)^4(\gamma-1)} \frac{R^2}{2t} \right) . \tag{2.14}$$

The main idea of the proof is that the numerator γ^{k+1} grows in k much faster than the denominator $(k+3)^4$ whenever $\gamma > 1$. In particular, there exists a positive number $m = m(\gamma)$ such that

$$\frac{\gamma^{k+1}}{(k+3)^4(\gamma-1)} \geq m(k+2) \tag{2.15}$$

for any $k \geq 0$. We can just take

$$m = \inf_{k \geq 0} \frac{\gamma^{k+1}}{(k+3)^4(k+2)(\gamma-1)}.$$

Let us denote for simplicity $L = \log A \frac{f(t_0)}{f(t_1)}$ and rewrite the inequality (2.14) as follows

$$\begin{aligned} I_R(t) &\leq \frac{1}{f(t)} \sum_{k=0}^{\infty} \exp\left((k+1)L - m(k+2)\frac{R^2}{2t} \right) \\ &= \frac{1}{f(t)} \exp\left(-m\frac{R^2}{2t} \right) \sum_{k=0}^{\infty} \exp\left(-(k+1)(m\frac{R^2}{2t} - L) \right) . \end{aligned}$$

We have either

$$m\frac{R^2}{2t} - L \geq \log 2$$

or

$$m\frac{R^2}{2t} - L < \log 2.$$

In the former case, we obtain obviously

$$\begin{aligned} I_R(t) \leq & \quad \frac{1}{f(t)} \exp\left(-m\frac{R^2}{2t} \right) \sum_{k=0}^{\infty} 2^{-(k+1)} \\ = & \quad \frac{1}{f(t)} \exp\left(-m\frac{R^2}{2t} \right) , \end{aligned} \tag{2.16}$$

while in the latter case we estimate $I_R(t)$ in a different way:

$$\begin{aligned} I_R(t) \le I(t) &\le \frac{1}{f(t)} \\ &\le \frac{1}{f(t)} \exp\left(L + \log 2 - m\frac{R^2}{2t} \right) \\ &= \frac{2}{f(t)} A \frac{f(t)}{f(t/\gamma)} \exp\left(-m\frac{R^2}{2t} \right) \\ &= \frac{2A}{f(t/\gamma)} \exp\left(-m\frac{R^2}{2t} \right). \end{aligned}$$

Combining this together with (2.16) yields finally for both cases:

$$I_R(t) \le \frac{2A}{f(t/\gamma)} \exp\left(-m\frac{R^2}{2t} \right).$$

q.e.d.

STEP 2. The purpose of this part of the proof is to show that for $D \ge D_1 \equiv 5D_0$ and all $t > 0$ we have

$$E_D(t) \le \frac{4A}{f(t/\gamma)}. \tag{2.17}$$

To that end, we split the integral

$$E_D(t) = \int_\Omega u^2(x,t) \exp\left(\frac{r^2(x)}{Dt} \right) dx$$

(where $r(x) \equiv \operatorname{dist}(x, K)$) into a series

$$\begin{aligned} E_D(t) &= \int_{\{r(x)\le R\}} u^2(x,t) \exp\left(\frac{r^2(x)}{Dt} \right) dx \\ &+ \sum_{k=0}^{\infty} \int_{\{2^k R \le r(x) \le 2^{k+1} R\}} u^2(x,t) \exp\left(\frac{r^2(x)}{Dt} \right) dx, \end{aligned} \tag{2.18}$$

where $R > 0$ is an arbitrary number.

The first integral on the right-hand side (2.18) is bounded from above by

$$\exp\left(\frac{R^2}{Dt} \right) \int_\Omega u^2(x,t) dx \le \frac{1}{f(t)} \exp\left(\frac{R^2}{Dt} \right). \tag{2.19}$$

The k-th term in the sum (2.18) is estimated from above by using Lemma 2.2 as

$$
\begin{aligned}
&\le \exp\left(\frac{4^{k+1}R^2}{Dt}\right)\int_{\Omega\setminus K^{2^kR}} u^2(x,t)dx \\
&\le \frac{2A}{f(t/\gamma)}\exp\left(\frac{4^{k+1}R^2}{Dt}-\frac{4^kR^2}{D_0t}\right) \\
&\le \frac{2A}{f(t/\gamma)}\exp\left(-\frac{4^kR^2}{Dt}\right),
\end{aligned}
\tag{2.20}
$$

where we have used $D_0 \le D/5$.

Combining (2.19) and (2.20), we obtain

$$
E_D(t) \le \frac{1}{f(t)}\exp\left(\frac{R^2}{Dt}\right) + \frac{2A}{f(t/\gamma)}\sum_{k=0}^{\infty}\exp\left(-\frac{4^kR^2}{Dt}\right),
\tag{2.21}
$$

We can choose R here arbitrarily. Let us define R to satisfy the identity $R^2/Dt = \log 2$ and deduce from (2.21):

$$
E_D(t) \le \frac{2}{f(t)} + \frac{2A}{f(t/\gamma)}\sum_{k=0}^{\infty}2^{-4^k} \le \frac{2+2A}{f(t/\gamma)},
$$

whence (2.17) follows since $A \ge 1$.

Remark. By taking another (more optimal) value for R, namely,

$$
R^2 = Dt\log(1+\sqrt{2A}),
$$

we could replace the coefficient $2+2A$ in the formula above by a better value $1+2\sqrt{2A}$.

STEP 3. Now we will finish the proof of Theorem 2.1. In view of the previous step, it suffices to consider the case $2 < D < D_1$. The integral maximum principle (Proposition 2.3) implies that for any $s > 0$ the integral

$$
\int_\Omega u^2(x,t)\exp\left(\frac{r^2(x)}{2(t+s)}\right)dx
$$

is decreasing in $t \in (0,\infty)$, where $r(x) = \operatorname{dist}(x,K)$. Therefore, for any $\tau \in (0,t)$,

$$
\int_\Omega u^2(x,t)\exp\left(\frac{r^2(x)}{2(t+s)}\right)dx \le \int_\Omega u^2(x,\tau)\exp\left(\frac{r^2(x)}{2(\tau+s)}\right)dx.
\tag{2.22}
$$

Given $t > 0$ and $D, 2 < D < D_1$, let us find suitable values of s, τ so that the left-hand side of (2.22) is equal to $E_D(t)$ while the right-hand side is to be equal to $E_{D_1}(\tau)$. To that end, we solve simultaneously the equations

$$\begin{cases} 2(t+s) = Dt, \\ 2(\tau+s) = D_1\tau, \end{cases}$$

and obtain $s = \frac{D-2}{2}t$ and $\tau = \frac{D-2}{D_1-2}t < t$. Therefore, for this value of τ, we have

$$E_D(t) \le E_{D_1}(\tau),$$

and applying the inequality

$$E_{D_1}(\tau) \le \frac{4A}{f(\tau/\gamma)}$$

known from the previous step of the proof, we get finally

$$E_D(t) \le \frac{4A}{f(\frac{D-2}{D_1-2}t/\gamma)}.$$

Thus, we have proved Theorem 2.1 with

$$\delta = \delta(D,\gamma) = \gamma^{-1}\min\left(1, \frac{D-2}{D_1-2}\right).$$

q.e.d.

3. Pointwise estimates of the heat kernel

On any smooth connected Riemannian manifold M, we define the heat kernel $p(x,y,t)$ as the smallest positive fundamental solution to the heat equation. It exists, is unique, and can be constructed as follows. Let us take an increasing sequence of pre-compact regions $\Omega_k \subset M, k = 1, 2, 3, ...$ which exhausts M, and in each Ω_k construct the Green function $p_k(x,y,t)$ to the Dirichlet problem for the heat equation. Then, on one hand, we have by the maximum principle

$$0 \le p_k \le p_{k+1},$$

while on the other hand

$$\int_{\Omega_k} p_k(x,y,t)dx \le 1.$$

These two properties ensure that there is a limit

$$p(x,y,t) \equiv \lim_{k\to\infty} p_k(x,y,t),$$

which is, by definition, the (minimal) heat kernel (see [14] for detailed justification of this construction).

If the manifold M has a boundary, then the exhausting regions Ω_k will necessarily have for large k a part of their boundary on ∂M, so one can put a boundary condition (normally Dirichlet or Neumann one) on ∂M to be satisfied by all p_k and, therefore, by $p(x,y,t)$.

Our main result is the following theorem.

Teorem 3.1. *Let x, y be two points on an arbitrary manifold M, and let us have for all $t > 0$*

$$p(x,x,t) \le \frac{1}{f(t)} \tag{3.1}$$

and

$$p(y,y,t) \le \frac{1}{g(t)}, \tag{3.2}$$

where f, g are regular functions in the sense of the previous section. Then for any $C > 4$ and all $t > 0$

$$p(x,y,t) \le \frac{4A}{\sqrt{f(\delta t) g(\delta t)}} \exp\left(-\frac{r^2(x,y)}{Ct}\right), \tag{3.3}$$

where $r(x,y) = \operatorname{dist}(x,y)$, $\delta = \delta(C,\gamma)$, and A, γ are the constants from (2.2).

Remark. The theorem is applicable also if the inequalities (3.1) and (3.2) hold only on a bounded time interval $(0,T)$ as stated in Theorem 1.1 in the Introduction (with an obvious modification of the notion of regularity for a bounded interval). Indeed, the on-diagonal heat kernel $p(x,x,t)$ is known to a decreasing function of t. Therefore, if we extend the functions $f(t)$ and $g(t)$ beyond the point T as constants, then (1.3) and (3.2) will be valid for all $t > 0$. Moreover, it is evident that the extended functions will preserve regularity, so that we can apply Theorem 3.1 and obtain (3.3), in particular, for all $t \in (0,T)$.

Proof of Theorem 3.1. Let us apply the following universal inequality which is true always:

(3.4)
$$p(x,y,t) \le \sqrt{E_D(x,t/2), E_D(y,t/2)} \exp\left(-\frac{r^2(x,y)}{2Dt}\right),$$

where D is a positive constant and

$$E_D(z,t) \equiv \int_M p^2(z,\zeta,t)\exp\left(\frac{r^2(z,\zeta)}{Dt}\right)\,d\zeta.$$

This inequality was proved in [18] but the proof is very short so that we can reproduce it here for the sake of completeness. Indeed, by the semigroup property of the heat kernel and by the triangle inequality $r^2(x,y) \le 2(r^2(x,z)+r^2(y,z))$ we have:

$$\begin{aligned} p(x,y,t) &= \int_M p(x,z,t/2)p(z,y,t/2)dz \\ &\le \int_M p(x,z,t/2)\exp\left(\frac{r^2(x,z)}{Dt}\right) \\ &\quad \times p(z,y,t/2)\exp\left(\frac{r^2(y,z)}{Dt}\right)\exp\left(-\frac{r^2(x,y)}{2Dt}\right)\,dz \\ &\le \exp\left(-\frac{r^2(x,y)}{2Dt}\right)\left(\int_M p^2(x,z,t/2)\exp\left(\frac{r^2(x,z)}{Dt/2}\right)\,dz\right)^{\frac{1}{2}} \\ &\quad \times \left(\int_M p^2(y,z,t/2)\exp\left(\frac{r^2(y,z)}{Dt/2}\right)\,dz\right)^{\frac{1}{2}} \\ &= \exp\left(-\frac{r^2(x,y)}{2Dt}\right)\left(E_D(x,t/2)E_D(y,t/2)\right)^{\frac{1}{2}}, \end{aligned}$$

what was to be proved.

The rest of the proof of Theorem 3.1 follows from

Theorem 3.2. *Let x be a point on an arbitrary manifold M, and let us have for all $t>0$*

$$p(x,x,t) \le \frac{1}{f(t)}, \tag{3.5}$$

where $f(t)$ is a regular function. Then for any $D>2$ and all $t>0$

$$E_D(x,t) \le \frac{4A}{f(2\delta t)}, \tag{3.6}$$

where $\delta=\delta(D,\gamma)$, and A,γ are the constants from (2.2).

To finish the proof of Theorem 3.1 we are left to notice that (3.1) and (3.2) imply (3.6) and a similar inequality for the point y, which together with (3.4) yield (3.3) (we have to replace in the final result $2D$ by C).

Proof of Theorem 3.2. Let us consider one of the sets Ω_k containing the point x. Since $p_k \le p$, the inequality (3.5) is valid for p_k, too. It is sufficient to show that (3.6) holds for the integral

$$E_{D,k}(x,t) \equiv \int_{\Omega_k} p_k^2(x,z,t) \exp\left(\frac{r^2(x,z)}{Dt} \right) dz,$$

since thereafter we could pass to the limit as $k \to \infty$ and establish the same upper bound for $E_D(x,t)$.

Let us apply Theorem 2.1 to estimate $E_{D,k}(x,t)$. Indeed, the function $u(z,t) \equiv p_k(x,z,t)$ satisfies the conditions (2.1) with the single-point compact $K = \{x\}$, and for this function we have

$$\begin{aligned} I(t) = \int_\Omega u^2(z,t)dz &= \int_\Omega p_k(x,z,t)p_k(z,x,t)dz \\ &= p_k(x,x,2t) \le \frac{1}{f(2t)}. \end{aligned}$$

Therefore, by Theorem 2.1 we obtain for any $D > 2$

$$E_{D,k}(x,t) = \int_\Omega u^2(z,t) \exp\left(\frac{r^2(x,z)}{Dt} \right) dz \le \frac{4A}{f(2\delta t)},$$

what was to be proved. q.e.d.

Theorem 3.2 may have other applications. For example, in conjunction with the result of [17] it can give upper bounds of derivatives of the heat kernel. Indeed, as proved in [17], any upper bound for $E_D(x,t)$

$$E_D(x,t) \le \frac{1}{h(t)},$$

which is supposed to be true for some x and all $t > 0$, implies

$$E_D^{(1)}(x,t) \equiv \int_M |\nabla_z p|^2 (x,z,t) \exp\left(\frac{r^2(x,z)}{Dt} \right) dz \le \frac{\mathrm{const}_D}{h^{(1)}(t)}$$

and

$$\begin{aligned} E_D^{(2)}(x,t) \equiv \;& \int_M |\Delta_z p|^2 (x,z,t) \exp\left(\frac{r^2(x,z)}{Dt} \right) dz \\ \le \;& \frac{\mathrm{const}_D}{h^{(2)}(t)}, \end{aligned} \tag{3.7}$$

where

$$h^{(1)}(t) = \int_0^t h(s)ds,$$
$$h^{(2)}(t) = \int_0^t h^{(1)}(s)ds,$$

and $D > 2$.

Another result of [17] is an inequality similar to (3.4)

(3.8)
$$\left|\frac{\partial p}{\partial t}\right|(x,y,t) \leq \sqrt{E_D^{(2)}(x,t/2), E_D(y,t/2)}\exp\left(-\frac{r^2(x,y)}{2Dt}\right).$$

Combinig together the inequalities (3.8), (3.7) and (3.6), we obtain the following statement.

Corollary 3.3. *Under hypotheses of Theorem 3.1 we have in addition to (1.5) also*

$$\left|\frac{\partial p}{\partial t}\right|(x,y,t) \leq \frac{\mathrm{const}_{A,C,\gamma}}{\sqrt{f^{(2)}(\delta t)g(\delta t)}}\exp\left(-\frac{r^2(x,y)}{Ct}\right),$$

provided $C > 4$.

Similar estimates can be proved also for the higher order time derivatives of the heat kernel.

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