Precise Gaussian estimates of heat kernels on asymptotically flat Riemannian manifolds with poles

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Abstract

We give precise Gaussian upper and lower bound estimates on heat kernels on Riemannian manifolds with poles under assumptions that the Riemannian curvature tensor goes to 0 sufficiently fast at infinity. Under additional assumptions on the curvature, we give estimates on the logarithmic derivatives of the heat kernels. The proof relies on the Elworthy-Truman's formula of heat kernels and Elworthy and Yor's observation on the derivative process of certain stochastic flows. As an application of them, we prove logarithmic Sobolev inequalities on pinned path spaces over such Riemannian manifolds.

1. Introduction

Let $p(t,x,y)$ be the heat kernel of a diffusion semigroup $e^{t\Delta/2}$ on a d-dimensional complete Riemannian manifold (M,g), where Δ denotes the Laplace-Beltrami operator on (M,g). For some classes of Riemannian manifolds, the following Gaussian upper and lower bounds are valid (see [30]): For all $t>0$, $x,y\in M$, it holds that

$$C_1 t^{-d/2}\exp\left(-\frac{d(x,y)^2}{2(1-C_2)t}\right)\le p(t,x,y)\le C_3 t^{-d/2}\exp\left(-\frac{d(x,y)^2}{2(1+C_4)t}\right), \tag{1.1}$$

where $d(x,y)$ denotes the Riemannian distance between x and y, C_1,C_3 are positive constants and C_2,C_4 are nonnegative constants with $C_2<1$. It is natural to expect that more precise estimate holds under stronger assumptions on the Riemannian manifold. In fact, under nonnegativity of the Ricci curvature, Li-Yau's lower bound estimate [24], (1.1) with $C_1=(2\pi)^{-d/2}, C_2=0$, holds. Also if the sectional curvature is nonpositive and M is simply connected, the upper bound in (1.1) holds with $C_3=(2\pi)^{-d/2}$ and $C_4=0$ by [7]. Note that the lower bound in (1.1) does not hold for $t\in[0,T]$ for any fixed T in the case of hyperbolic spaces. In [2], the author proved the lower bound with $C_2=0$ for any $t\in[0,T]$ under the assumptions that x is a pole and the derivatives of Riemannian metric go to 0 sufficiently fast at infinity although negative curvature part remains. In this paper, we prove similar estimates on Riemannian manifolds with poles under the assumptions that the curvature and the derivatives go to 0 sufficiently fast at infinity. The present proof is simpler than the previous one. Also we discuss estimates on the logarithmic derivatives of heat kernels. The second derivative of $\log p(t,x,y)$ with respect to y was studied in connection with parabolic Harnack inequality [24], [32]. On the other hand, it is pointed out in [18], [22] that $\nabla_y^2\log p(t,x,y)$ is related to a logarithmic Sobolev inequality (=LSI for short) on loop space over the Riemannian manifold. In [1], sufficient conditions for LSI in terms of the heat kernel were given. Malliavin and Stroock [25] showed that the small time behavior of the second derivative of $\log p(t,x,y)$ dramatically changes if y is in the cut-locus of x. However in our case, there are no cut-locus and we can check the conditions in [1] by our main theorem. The key ingredients of our arguments are the Elworthy and Truman's formula [15] and Elworthy and Yor's observation on the derivative process of stochastic flows [16]. In [29], Ndumu studied derivative formulae of heat kernels by using Elworthy and Truman's formula. However, his assumptions on the boundedness of the derivative process is too restrictive. The key point in the present paper is to use Elworthy and Yor's observation to avoid the difficulty.

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2. Elworthy and Truman's formula and estimates on heat kernels

Let (M,g) be a d-dimensional complete Riemannian manifold with a pole o. That is, we assume that the exponential map $\exp : T_oM \to M$ is a diffeomorphism. Let

$$\theta(x) = \det\left[(d\exp_o)_{\exp_o^{-1}(x)}\right], \tag{2.1}$$

where $(d\exp_o)_{\exp_o^{-1}(x)}$ denotes the derivative of the exponential map at $\exp_o^{-1}(x)$. Note that θ is a positive smooth function on M. This is called a Ruse's invariant. Now, we embed M into a higher dimensional Euclidean space $\mathbb{R}^N$ isometrically and let $P(x) : \mathbb{R}^N \to T_xM$ be the projection operator. Let us consider the following SDE with a singular drift at time t:

$$\begin{aligned} dX(s,x,w) &= b_s\left(X(s,x,w)\right)ds + P\left(X(s,x,w)\right)\circ dw(s) \quad (0\le s<t) && (2.2)\\ X(0,x,w) &= x, && (2.3)\end{aligned}$$

where

$$b_s(x) = -\frac{1}{t-s}\nabla\left(\frac{d(o,x)^2}{2}\right) - \frac{1}{2}\nabla\log\theta(x). \tag{2.4}$$

For simplicity, we denote $E(x) = d(o,x)^2/2$ sometimes. Let $p(t,x,y)$ be the heat kernel of $e^{t\Delta/2}$. Elworthy-Truman [15], [12] proved that

THEOREM 2.1. (1) *$X(s,x,w)$ $(0\le s<t)$ exists for almost all w and* $\lim_{s\to t} X(s,x,w) =$ *o. Also the law of the process $d(o,X(s,x,w))$ is the same as that of the radial part of the pinned Brownian motion on $\mathbb{R}^d$ which starts at a point whose Euclidean norm is $d(o,x)$ and arrives at the origin at time t.*
(2) *For any x, it holds that*

$$p(t,o,x) \;=\; \frac{\exp\left(-\frac{d(o,x)^2}{2t}\right)}{(2\pi t)^{d/2}}\theta(x)^{-1/2}h(t,o,x), \tag{2.5}$$

where

$$h(t,o,x) := E\left[\exp\left(\int_0^t V\left(X(s,x,w)\right)ds\right)\right], \tag{2.6}$$

$$V(x) = \frac{1}{2}\theta(x)^{1/2}\Delta\left(\theta^{-1/2}\right)(x). \tag{2.7}$$

To state our estimates, we recall basic notions in Riemannian geometry. Let $R(X,Y)Z := \nabla_X\nabla_Y Z - \nabla_Y\nabla_X Z - \nabla_{[X,Y]}Z$ be the Riemannian curvature tensor, where X, Y, Z are vector fields on M. The Ricci curvature, $\mathrm{Ric}_x \in T_xM^* \otimes T_xM$ is given by $\mathrm{Ric} = \sum_{i=1}^d R(\cdot, e_i)e_i$, where $\{e_i\}$ is an orthonormal frame of T_xM. Let K be the sectional curvature, that is $K_\pi(x) = g(R(X,Y)(Y),X)$, where $X, Y \in T_xM$ are orthogonal unit vectors and π is the plane spanned by X, Y. We consider the following assumption. We identify a second covariant derivative of a function with a symmetric operator below.

Assumption 2.2. (A1) *The n-th covariant derivatives of* $\log\theta(x)$ $(1 \le n \le 4)$ *are bounded continuous functions on M.*
(A2) *There exists a positive constant $\varepsilon > 0$ such that for all $x \in M$,*

$$\nabla_x^2\left\{\frac{d(o,x)^2}{2}\right\} \ge \frac{1+\varepsilon}{2}I_{T_xM}. \tag{2.8}$$

(A3) *There exists a constant $C > 0$ such that for all $x \in M$,*

$$\left\|\nabla_x^3\left\{\frac{d(o,x)^2}{2}\right\}\right\| + \left\|\nabla_x^2\left\{\frac{d(o,x)^2}{2}\right\}\right\| \le C. \tag{2.9}$$

(A4) *The Riemannian curvature tensor and the first derivative of the Ricci curvature are bounded.*

By using the Levi-Civita connection, the semimartingale $X(s,x,w)$ $(0 \le s < t)$ can be lifted to the orthonormal frame bundle $O(M)$ and stochastic parallel translation $\tau(X)_s : T_xM \to T_{X(s,x,w)}M$ can be defined. Any tensor T on $T_{X(t,x,w)}M$ can be parallel translated to a tensor $\overline{T(X)}_t$ on T_xM along X. We use this notation frequently. The following derivative formulae are keys in our argument. The formulae (2.10) and (2.11) hold under weaker assumptions. However, we do not intend to refine the results in this paper.

Lemma 2.3. *Assume* (A1), (A2), (A3), (A4).*Then the following formulae hold:*

$$\begin{aligned} &\nabla_x h(t,o,x)(\xi) \\ &= E\left[\int_0^t \left(\overline{\nabla V(X)}_s, \bar{v}_1(\xi,s)\right)ds \cdot \exp\left(\int_0^t V\left(X(s,x,w)\right)ds\right)\right] \end{aligned} \tag{2.10}$$

$$
\begin{aligned}
(2.11)\quad & \nabla_x^2 h(t,o,x)(\xi_1,\xi_2) \\
&= E\Bigg[\Bigg\{\int_0^t \left(\overline{(\nabla V)(X)}_s, \bar{v}_2(\xi_1,\xi_2,s) - \int_0^s \overline{R(X)}_u(\bar{v}_1(\xi_2,u), \circ d\overline{X}(u))\bar{v}_1(\xi_1,s)\right) ds \\
&+ \int_0^t \overline{(\nabla^2 V)(X)}_s(\bar{v}_1(\xi_1,s),\bar{v}_1(\xi_2,s))ds \\
&+ \int_0^t \left(\overline{(\nabla V)(X)}_s, \bar{v}_1(\xi_1,s)\right) ds \int_0^t \left(\overline{(\nabla V)(X)}_s, \bar{v}_1(\xi_2,s)\right) ds\Bigg\} \\
&\qquad \times \exp\left(\int_0^t V\left(X(s,x,w)\right) ds\right)\Bigg]
\end{aligned}
$$

where $\xi, \xi_1, \xi_2 \in T_xM$ and $\bar{v}_1(\cdot,s) \in T_xM^* \otimes T_xM$, $\bar{v}_2(\cdot,\cdot,s) \in T_xM^* \otimes T_xM^* \otimes T_xM$ are the solutions to the following ODEs:

$$
\begin{aligned}
(2.12)\qquad \dot{\bar{v}}_1(\xi,s) &= \left\{-\frac{1}{t-s}\overline{\nabla^2 E(X)}_s - \frac{1}{2}\overline{\mathrm{Ric}(X)}_s - \frac{1}{2}\overline{\nabla^2 \log\theta(X)}_s\right\}\bar{v}_1(\xi,s) \\
\bar{v}_1(\xi,0) &= \xi
\end{aligned}
$$

$$
\begin{aligned}
(2.13)\qquad & \dot{\bar{v}}_2(\xi_1,\xi_2,s) \\
&= \left\{-\frac{1}{t-s}\overline{\nabla^2 E(X)}_s - \frac{1}{2}\overline{\mathrm{Ric}(X)}_s - \frac{1}{2}\overline{\nabla^2 \log\theta(X)}_s\right\}\bar{v}_2(\xi_1,\xi_2,s) \\
&+ \int_0^s \overline{R(X)}_u\left(\bar{v}_1(\xi_2,u), \circ d\overline{X}(u)\right)\Bigg\{-\frac{1}{t-s}\overline{\nabla^2 E(X)}_s - \frac{1}{2}\overline{\mathrm{Ric}(X)}_s \\
&- \frac{1}{2}\overline{\nabla^2 \log\theta(X)}_s\Bigg\}\bar{v}_1(\xi_1,s) - \frac{1}{t-s}\overline{\nabla^3 E(X)}_s(\bar{v}_1(\xi_1,s),\bar{v}_1(\xi_2,s)) \\
&- \frac{1}{2}\overline{\nabla \mathrm{Ric}(X)}_s(\bar{v}_1(\xi_1,s),\bar{v}_1(\xi_2,s)) - \frac{1}{2}\overline{\nabla^3 \log\theta(X)}_s(\bar{v}_1(\xi_1,s),\bar{v}_1(\xi_2,s)) \\
\bar{v}_2(\xi_1,\xi_2,0) &= 0
\end{aligned}
$$

and $\overline{X}(s) = \int_0^s \tau(X)_s^{-1} \circ dX(s,x,w)$. Moreover, $V, \nabla V, \nabla^2 V$ and $\sup_{0\le s\le t}\|\bar{v}_1(t)\|_{op}$ are bounded functions of x and w. Also $\sup_x E\left[\sup_{0\le s\le t}\|\bar{v}_2(s)\|_{op}^p\right] < \infty$ for all $p > 1$. In particular, $\nabla_x h(t,o,x), \nabla_x^2 h(t,o,x)$ are bounded functions on M.

Proof. Note that

$$V(x) = \frac{1}{4}\left(|\nabla \log\theta(x)|^2 - 2\Delta\log\theta(x)\right).$$

Hence, (A1) implies V, ∇V, $\nabla^2 V$ are bounded. Let $N(x) : \mathbb{R}^d \to T_xM^\perp$ be the projection operator. We also fix a metric connection on the normal bundle $\pi : N(M) \to M$. Let

$$
\begin{aligned}
(2.14)\qquad b(s) &= \int_0^s \left\{\tau(X)_s^{-1} P(X(s,x,w)\right\} \circ dw(s) \\
(2.15)\qquad \beta(s) &= \int_0^s \left\{\tau(X)_s^{-1} N(X(s,x,w)\right\} \circ dw(s)
\end{aligned}
$$

Note that $b(s)$ and $\beta(s)$ are independent Brownian motions on T_xM and $T_xM^{\perp}$ respectively. Since $\overline{X}(s)$ satisfies the following SDE,

$$\begin{aligned} d\overline{X}(s) &= -\frac{1}{t-s}\overline{\nabla E(X)}_s ds - \frac{1}{2}\overline{\nabla \log\theta(X)}_s ds + db(s), && (2.16)\\ \overline{X}(0) &= 0, && (2.17) \end{aligned}$$

$\overline{X}(s)$ and $X(s,x,w)$ are $\mathfrak{B}$-measurable, where $\mathfrak{B} = \sigma(b(s) \mid 0 \le s < 1)$. Note that, formally, $v_1(\xi,s) = \tau(X)_s^{-1}\partial_x X(s,x,w)(\xi)$ satisfies the following SDE:

$$\begin{aligned} dv_1(\xi,s) &= \overline{A(X)}_s(v_1(\xi,s),d\beta(s)) - \frac{1}{2}\overline{\mathrm{Ric}(X)}_s(v_1(\xi,s)) && (2.18)\\ &\quad -\frac{1}{t-s}\overline{\nabla^2 E(X)}_s(v_1(\xi,s)) - \frac{1}{2}\overline{\nabla^2\log\theta(X)}_s(v_1(\xi,s))\\ v_1(\xi,0) &= \xi, \end{aligned}$$

where A denotes the shape operator of M in $\mathbb{R}^N$. The non-explosion property of X implies that $X(s,x,w)$ exists for all $0<s<t$. However, in noncompact cases, we cannot expect the existence of a differentiable version of $X(s,x,w)$ with respect to x even if the coefficient of SDE is smooth and conservative. See [33] and references in it. In the case of compact manifolds, there is a version such that for almost all w and all $s>0$, $x \to X(s,x,w)$ is a diffeomorphism and (2.18) holds. See [16], [4]. Roughly speaking, (2.12) can be obtained by taking the conditional expectation of $v_1(\xi,s)$ with respect to $\mathfrak{B}$ by noting the independence of $\mathfrak{B}$ and β. Similarly (2.10) can be proved by taking the conditional expectation with respect to $\mathfrak{B}$ in the Wiener functional representation formula for $\nabla_x h(t,o,x)$ which is obtained by taking the derivative of (2.6) with the help of (2.18) and (2.12) as in [16], [4], [13].

However $\overline{A(X)}_s$ may not be integrable function on the Wiener space and so we should be careful to take derivative and the conditional expectation. Hence, we need consider the approximate function of $h(t,o,x)$ to differentiate itself. Let

$$\begin{aligned} &h_{\varepsilon,L}(t,o,x) && (2.19)\\ &\quad = E\left[\exp\left(\int_0^{t-\varepsilon} V\left(X(s,x,w)\right)ds\right)\varphi_L\left(\|d(o,X(\cdot,x,w))^2\|^{2m}_{\kappa,m,t-\varepsilon}\right)\right]. \end{aligned}$$

Here φ_L is a smooth cut-off function whose support is in $[-L^2,L^2]$ and $\varphi(u)=1$ for $u\in[-L,L]$ and all derivatives of φ_L goes to 0 uniformly on $\mathbb{R}$ when $L\to\infty$. $\|\ \|_{\kappa,m,t}$ is given by

$$\|\gamma\|^{2m}_{\kappa,m,t} = \|\gamma\|^{2m}_{L^{2m}([0,t])} + \int_0^t\int_0^t \frac{|\gamma(u)-\gamma(s)|^{2m}}{|u-s|^{1+2m\kappa}}duds,$$

where $0<\kappa<1/2, 2\kappa m>1$ and m is an integer. Note that the norm $\|\ \|_{\kappa,m,t}$ can be defined for positive real number m satisfying the above relation on m and κ. Then $\lim_{\varepsilon\to0,L\to\infty} h_{\varepsilon,L}(t,o,x) = h(t,o,x)$. In (2.19), we may assume $X(s,x,w)$ is smooth with respect to x because we may assume $X(\cdot,x,w)$ moves in a compact subset thanks to the existence of the cut-off function. Thus we can differentiate both sides of (2.19) and we may assume that the equation (2.18) is valid up to the exit time of $X(s,x,w)$ from a compact set. Consequently, we have

$$
\begin{aligned}
(2.20)\qquad & (\nabla h_{\varepsilon,N}(t,o,x),\xi) \\
&= E\Bigg[\left(\int_0^{t-\varepsilon}\left(\overline{\nabla V(X)}_s, v_1(\xi,s)\right)ds\right)\exp\left(\int_0^{t-\varepsilon} V\left(X(s,x,w)\right)ds\right) \\
&\qquad\qquad \times\varphi_L\left(\|d(o,X(\cdot,x,w))^2\|^{2m}_{\kappa,m,t-\varepsilon}\right)\Bigg] \\
&\quad + E\left[\exp\left(\int_0^{t-\varepsilon} V\left(X(s,x,w)\right)ds\right)\varphi_L'(\|d(o,X(\cdot,x,w))^2\|^{2m}_{\kappa,m,t-\varepsilon})\Phi_1(\xi,w)\right],
\end{aligned}
$$

where

$$
\begin{aligned}
(2.21)\qquad \Phi_1(\xi,w) &= 4m\int_0^{t-\varepsilon} d(o,X(s,x,w))^{4m-1}\left(\overline{\nabla d(o,X)}_s, v_1(\xi,s)\right)ds \\
&\quad +4m\int_0^{t-\varepsilon}\int_0^{t-\varepsilon}\frac{\{d(o,X(u,x,w))^2-d(o,X(s,x,w))^2\}^{2m-1}}{|u-s|^{1+2m\kappa}} \\
&\quad \cdot\left\{\left(\overline{\nabla E(X)}_u, v_1(\xi,u)\right)-\left(\overline{\nabla E(X)}_s, v_1(\xi,s)\right)\right\}duds.
\end{aligned}
$$

If $X(s,x,w)$ moves in a compact subset in (2.20), (2.21), $\overline{A(X)}_s$ are bounded and so it holds that for all $1\le p<\infty$ and $0<l<\infty$,

$$
(2.22)\qquad E\left[\sup_{0\le s\le t-\varepsilon}\|v_1(\xi,s)\|^p \ :\ \sup_{0\le s\le t-\varepsilon} d(o,X(s,x,w))<l\right]<\infty.
$$

Therefore $\sup_{0\le s\le t-\varepsilon}\|v_1(\xi,s)\|^p$ is integrable in (2.20) and (2.21) for all $1\le p<\infty$. Since

$$
\begin{aligned}
\Phi_1(\xi,w) &\le 4m\|d(o,X(\cdot,x,w))\|^{4m-1}_{L^{4m-1}([0,t-\varepsilon])}\sup_{0\le s\le t-\varepsilon}\|v_1(\xi,s)\| \\
&\quad +4Cm\|d(o,X(\cdot,x,w))^2\|^{2m}_{2m\kappa/(2m-1),m-(1/2),t-\varepsilon}\sup_{0\le s\le t-\varepsilon}\|v_1(\xi,s)\|,
\end{aligned}
$$

we can take conditional expectation with respect to $\mathfrak{B}$ in (2.20). Then we can replace $v_1(\xi,s)$ by $\bar v_1(\xi,s)$ in (2.20) which we call equation (2.20)'. If the boundedness of $\bar v_1$ can be proved, by taking the limit $\varepsilon\to 0, L\to\infty$, we obtain (2.10). By taking derivative with respect to x in (2.20)', (2.11) follows from the same argument as (2.10) noting that

$$
(2.23)\qquad \left(\nabla_x\overline{T(X)}_s,\xi\right)=\left(\overline{\nabla T(X)}_s, v_1(\xi,s)\right)+\int_0^s\overline{R(X)}_u\left(v_1(\xi,u),\circ d\overline{X}(u)\right)\overline{T(X)}_s.
$$

Now we need only to prove the boundedness of $\bar v_i$. Let

$$
(2.24)\qquad C(X)_s=\overline{\nabla^2 E(X)}_s-\alpha I_{T_xM},
$$

where α is a positive number such that $\frac{1}{2}<\alpha<\frac{1+\varepsilon}{2}$. Note that $C(X)_s$ is a positive symmetric operator. Let $N(X)_s$ be the $T_xM^*\otimes T_xM$-valued process such that

$$
\begin{aligned}
(2.25)\qquad \dot N(X)_s &= \left\{-\frac{C(X)_s}{t-s}-\frac{1}{2}\overline{\mathrm{Ric}(X)}_s-\frac{1}{2}\overline{\nabla^2\log\theta(X)}_s\right\}N(X)_s \\
(2.26)\qquad N(X)_0 &= I
\end{aligned}
$$

Then $\bar{v}_1(\xi,s)=(t-s)^{\alpha}\overline{N(X)}_s\xi$. Also explicitly, we have

$$\begin{aligned}\bar{v}_2(\xi_1,\xi_2,s) &= (t-s)^{\alpha}\int_0^s (t-u)^{-\alpha}N(X)_sN(X)_u^{-1}\Bigg[-\frac{1}{t-u}\overline{\nabla^3E(X)}_u(\bar{v}_1(\xi_1,u),\bar{v}_1(\xi_2,u))\\ &\quad -\frac{1}{2}\overline{\nabla\mathrm{Ric}(X)}_u(\bar{v}_1(\xi_1,u),\bar{v}_1(\xi_2,u))-\frac{1}{2}\overline{\nabla^3\log\theta(X)}_u(\bar{v}_1(\xi_1,u),\bar{v}_1(\xi_2,u))\\ &\quad +\int_0^u\overline{R(X)}_\tau\left(\bar{v}_1(\xi_2,\tau),\circ d\overline{X}(\tau)\right)\Big\{-\frac{1}{t-u}\overline{\nabla^2E(X)}_u-\frac{1}{2}\overline{\mathrm{Ric}(X)}_u\\ &\quad -\frac{1}{2}\overline{\nabla^2\log\theta(X)}_u\Big\}\bar{v}_1(\xi_1,u)\Bigg]du.\end{aligned}$$

Since $\sup_{0\le u\le s\le t}\|N(X)_sN(X)_u^{-1}\|\le C$ (see Lemma 3.2 in [1]), $\|\bar{v}_1(\xi,s)\|\le C(t-s)^{\alpha}$. Also by the boundedness of the Riemannian curvature tensor and ∇^2E, we can complete the proof of the uniform boundedness of L^p-norm of $\bar{v}_2$. □

We introduce a function $\varphi_a(t)$ for $a\ge 0$ such that

$$\varphi_a(t)=\begin{cases}\frac{e^{\sqrt{a}t}-1}{\sqrt{a}} & \text{if } a>0\\ t & \text{if } a=0\end{cases}$$

The following are our main estimates.

Theorem 2.4. *We assume that*

$$-a:=\inf_{x,\pi}K_\pi(x)>-\infty \tag{2.27}$$

and $a\ge 0$. We denote

$$R_n(t) = \sup\left\{\|\nabla^kR(x)\| \;\Big|\; d(o,x)=t, 0\le k\le n\right\}. \tag{2.28}$$

(1) *Further we assume that*

$$\delta:=\int_0^\infty \varphi_a(t)R_0(t)dt < 1. \tag{2.29}$$

Then for any $x\in M$,

$$\frac{1-\delta}{1+\delta}I_{T_xM}\le\nabla_x^2\left\{\frac{d(o,x)^2}{2}\right\}\le\frac{1+\delta}{1-\delta}I_{T_xM}. \tag{2.30}$$

(2) *Assume* (2.29) *and*

$$\int_0^\infty\varphi_a(t)t^2R_2(t)dt<\infty. \tag{2.31}$$

Then it holds that $0<\inf\theta(x)\le\sup\theta(x)<\infty$, $\sup|\nabla^n\theta(x)|<\infty$ *for* $n=1,2$ *and*

$$\sup_x\left\|\nabla_x^3\left\{\frac{d(o,x)^2}{2}\right\}\right\|<\infty. \tag{2.32}$$

(3) *Assume the same assumptions as in* (2). *Set*

$$f(t,x) = (2\pi t)^{d/2} \exp\left(\frac{d(o,x)^2}{2t}\right) p(t,o,x). \tag{2.33}$$

Then for fixed $0 < T < \infty$, *there exist positive constants* $C_1(T) < C_2(T)$ *such that for all* $x \in M$, $0 < t \le T$,

$$C_1(T) \le f(t,x) \le C_2(T). \tag{2.34}$$

(4) *Assume* (2.29) *with* $\delta < 1/3$ *and*

$$\int_0^\infty \varphi_a(t) t^4 R_4(t) dt < \infty. \tag{2.35}$$

Then there exists positive constant $C_3(T)$ *such that*

$$\sup_{0<t\le T, x\in M} \|\nabla_x^k f(t,x)\| \le C_3(T), \tag{2.36}$$

where $k = 1, 2$.

When $a = 0$, that is, M is a nonnegative curvature manifold, by the results in [7, 24], the lower bound estimate in (2.34) holds with $C_1(T) = 1$. Note that $\inf_{x,\pi} K_\pi(x) \le 0$ because M is noncompact. If M is a nonpositive curvature manifold, all points of M are poles and we can prove the following.

Corollary 2.5. *Assume*

$$-\infty < -a := \inf_{x,\pi} K_\pi(x) \le \sup_{x,\pi} K_\pi(x) \le 0. \tag{2.37}$$

Let us fix a point $p \in M$ *and set*

$$S_n(t) = \sup\left\{ \|\nabla^k R(x)\| \;\middle|\; d(p,x) \ge t, 0 \le k \le n \right\}. \tag{2.38}$$

(1) *Further we assume that*

$$\int_0^\infty \varphi_a(t) S_0(t) dt \quad < \quad \infty. \tag{2.39}$$

Then there exists a positive constant C *such that for any* $x, y \in M$,

$$I_{T_yM} \le \nabla_y^2 \left\{ \frac{d(x,y)^2}{2} \right\} \le C \cdot I_{T_yM}. \tag{2.40}$$

(2) *Assume*

$$\int_0^\infty \varphi_a(t) t^2 S_2(t) dt < \infty. \tag{2.41}$$

Then it holds that $0 < \inf_{x,y} \theta_x(y) \le \sup_{x,y} \theta_x(y) < \infty$, $\sup_{x,y} |\nabla_y^n \theta_x(y)| < \infty$ $(n = 1, 2)$ *and*

$$\sup_{x,y} \left\| \nabla_y^3 \left\{ \frac{d(x,y)^2}{2} \right\} \right\| < \infty.$$

Here $\theta_x(y)$ *denotes the Ruse's invariant in the case where the pole is* x.

(3) *Assume the same assumptions as in* (2). *Set*

$$f(t,x,y)=(2\pi t)^{d/2}\exp\left(\frac{d(x,y)^2}{2t}\right)p(t,x,y). \tag{2.42}$$

Then for fixed $0<T<\infty$, *there exists a positive constant* $D_1(T)<D_2(T)$ *such that for all* $x,y\in M$, $0<t\le T$,

$$D_1(T)\le f(t,x,y)\le D_2(T). \tag{2.43}$$

(4) *Assume*

$$\int_0^\infty \varphi_a(t)t^4S_4(t)dt<\infty. \tag{2.44}$$

Then there exists positive constants $D_3(T)$ *such that*

$$\sup_{0<t\le T,x,y\in M}\|\nabla_y^k f(t,x,y)\|\le D_3(T), \tag{2.45}$$

where $k=1,2$.

In the above corollary, if $a=0$, then M is a Euclidean space and all estimates are trivial. Note that assumptions (2.39), (2.41), (2.44) does not depend on the choice of p. Now we prove the above theorem and the corollary.

Proof of Theorem 2.4. Below, we proceed as if $a>0$. When $a=0$, the proof works by replacing a by a positive number ε first and taking the limit $\varepsilon\to 0$. Take $\xi\in T_oM$ and let $l_\xi(s)=\exp_o(s\xi)$. For $v_1,v_2\in T_oM$, let $J(s,v_1,v_2)$ be the solution to the following Jacobi equation:

$$\ddot{J}(s)=-\overline{R(l_\xi)}_s(J(s),\xi)(\xi),\quad J(0)=v_1,\quad \dot{J}(0)=v_2. \tag{2.46}$$

$J(s,0,v)$ has the following explicit form:

$$J(s,0,v)=s\cdot\tau(l_\xi)_s^{-1}\left((d\exp_o)_{s\xi}(v)\right). \tag{2.47}$$

Here we use the identification $T_{s\xi}(T_oM)=T_oM$. By the definition, we have $\theta(l_\xi(1))=\det J(1,0,\cdot)$ and we see

$$\overline{\nabla^2E(l_\xi)}_1\left(J(1,0,v),J(1,0,v)\right)=\left(\dot{J}(1,0,v),J(1,0,v)\right). \tag{2.48}$$

Thus if $v\to J(s,0,v)$ is invertible, then $\overline{\nabla^2E(l_\xi)}_1=\dot{J}(1,0,J^{-1}(1,0,\cdot))$. Hence, we give estimates on $J,\dot{J}$. Let $U(s)=J(s,0,v)$ and $V(s)=\frac{\dot{U}(s)}{\sqrt{a}\|\xi\|}$. Then $\rho(s)=\|U(s)\|^2+\|V(s)\|^2$ satisfies

$$\dot\rho(s)\;=\;2\sqrt{a}\|\xi\|\left((U(s),V(s))-\left(a^{-1}\overline{R(l_\xi)}_t(U(s),\frac{\xi}{\|\xi\|})\frac{\xi}{\|\xi\|},V(s)\right)\right). \tag{2.49}$$

Since $T(X,Z)=(R(X,Y)Y,Z)$ is a symmetric form of X,Z, $(R(X,Y)Y,Z)\ge -a\|X\|\|Z\|$ holds when $\|Y\|=1$. Therefore, we have $\dot\rho(s)\le 2\sqrt{a}\|\xi\|\rho(t)$ and

$$\max\{\|U(s)\|,\|V(s)\|\}\le\sqrt{\rho(s)}\le\frac{\exp(\sqrt{a}\|\xi\|s)}{\sqrt{a}\|\xi\|}\|v\|. \tag{2.50}$$

Also by the definition of $U(s)$, we have

$$\|J(s,0,v)\| = \|U(s)\| = \sqrt{a}\|\xi\| \int_0^s \|V(u)\| du \le \frac{\exp(\sqrt{a}\|\xi\|s) - 1}{\sqrt{a}\|\xi\|}\|v\|. \tag{2.51}$$

Moreover by the definition, we have

$$\begin{aligned} \|\dot{J}(s,0,v) - v\| &\le \int_0^s \|\overline{R(l_\xi)}_s(U(s),\xi)(\xi)\| ds \\ &\le \int_0^s R_0(\|\xi\|u)\|\xi\|^2 \frac{\exp(\sqrt{a}\|\xi\|u) - 1}{\sqrt{a}\|\xi\|}\|v\| du \\ &\le \int_0^{\|\xi\|s} R_0(u)\varphi_a(u) du \|v\|. \end{aligned} \tag{2.52}$$

This implies $(1-\delta)\|v\| \le \|\dot{J}(s,0,\cdot)\| \le (1+\delta)\|v\|$. By this, we have for all $s > 0$,

$$\|J(s,0,v) - sv\| \le s\int_0^\infty R_0(u)\varphi_a(u) du \|v\| \tag{2.53}$$

and $\|J(s,0,v) - sv\| \le s\delta\|v\|$. This implies $\{s(1+\delta)\}^{-1} \le \|J(s,0,\cdot)^{-1}\| \le \{s(1-\delta)\}^{-1}$. These prove (2.30). Since $\theta(l_\xi(1)) = \det J(1,0,\cdot)$, $\theta(\cdot)$ is bounded from below and above by positive constants. Next we prove the bound on $\nabla\theta, \nabla^2\theta$ in (2). To this end, differentiating the Jacobi equation for $U(s)$ with respect to ξ, we get an equation for $U_1(s) := \partial_\xi U(s)$ such that

$$\ddot{U}_1(s)(\cdot) = -\overline{R(l_\xi)}_s(U_1(s)(\cdot),\xi)(\xi) + W(s,v), \tag{2.54}$$

where $U_1(0) = \dot{U}_1(0) = 0$ and

$$\begin{aligned} W(s,v) = &-\overline{\nabla R(l_\xi)}_s(J(s,0,\cdot),U(s),\xi)(\xi) \\ &- \left(\int_0^s \overline{R(l_\xi)}_u(J(u,0,\cdot),\xi) du\right) \overline{R(l_\xi)}_s(U(s),\xi)(\xi) \\ &- \overline{R(l_\xi)}(U(s),\cdot)(\xi) - \overline{R(l_\xi)}(U(s),\xi)(\cdot). \end{aligned}$$

We represent $U_1(s)$ by the method of constant variation. To this end, for $t,\tau \ge 0$, let

$$K_\tau(t) = \begin{pmatrix} 0 & I \\ -\overline{R(l_\xi)}_{t+\tau}(\cdot,\xi)\xi & 0 \end{pmatrix}. \tag{2.55}$$

Let us consider the following ODE:

$$\dot{Q}(t) = K_\tau(t)Q(t) \tag{2.56}$$

$$Q(0) = I. \tag{2.57}$$

We denote the solution by $Q_\tau(t)$. Noting that $Q_0(t)Q_0^{-1}(s) = Q_s(t-s)$ for $t \ge s$, we have

$$\begin{aligned} \begin{pmatrix} U_1(s) \\ \dot{U}_1(s) \end{pmatrix} &= Q_0(t)\int_0^t Q_0(s)^{-1} \begin{pmatrix} 0 \\ W(s,v) \end{pmatrix} ds \\ &= \int_0^t Q_s(t-s) \begin{pmatrix} 0 \\ W(s,v) \end{pmatrix} ds \end{aligned} \tag{2.58}$$

We denote the first component of $Q_s(t)^t(0,v)$ by $J_s(t,0,v)$. Then, by the same method as in the case of $J(s,0,v)$, we have

$$\|J_s(t,0,v)\| \le Ct\|v\|. \tag{2.59}$$

Note that there exists a constant C which is independent of ξ such that $\int_0^1 |W(s,v)|ds \le C\|v\|$. For example,

$$\begin{aligned} \int_0^1 \left\|\overline{\nabla R(l_\xi)}_s(J(s,0,\cdot),U(s),\xi)(\xi)\right\| ds &\le \int_0^1 R_1(s\|\xi\|)\cdot Cs\cdot\frac{e^{\sqrt{a}\|\xi\|s}-1}{\sqrt{a}}\|\xi\|ds \\ &= \int_0^{\|\xi\|} sR_1(s)\varphi_a(s)ds. \end{aligned} \tag{2.60}$$

Other terms are also estimated in similar way. This implies $\sup_{0\le s\le 1}\|U_1(s)\| \le C\|v\|$, where C does not depend on ξ. Noting $U_1(s) = \overline{\nabla J(s,0,v)(J(s,0,))}$, we get for any $0 \le s \le 1$, $\sup_\xi \|\overline{\nabla J(s,0,v)}\| < \infty$. This implies $\nabla\theta$ is bounded. By the calculation similar to this, we obtain the boundedness of $\nabla^2\theta$ under (2.31). We prove (2.32). Noting

$$\partial_\xi\overline{\nabla^2 E(l_\xi)}_1 = \overline{\nabla^3 E(l_\xi)}_1(\cdot,\cdot,J(1,0,\cdot)),$$

we need only to prove $\sup_\xi \|\partial_\xi\left(\dot{J}(1,0,J^{-1}(1,0,\cdot))\right)\| < \infty$. This follows from the formula for $\dot{U}_1$ and estimates on $W(s,v)$, $\dot{J}_s(t-s,0,v)$. The estimate on $\dot{J}_s(t-s,0,v)$ is similar to that of $\dot{J}(t-s,0,v)$. We prove (3). If (2.29) holds with $\delta < 1/3$, then (A2) holds. By (2) and the explicit expression of V in terms of θ, (3) is obvious. For the proof (2.36), it suffices to prove that $\nabla^3\theta, \nabla^4\theta$ are bounded. To this end, it is sufficient to prove that $U_i(s) = \partial_\xi^i U(s)$ are matrices valued functions for $i = 3,4$ satisfying that

$$\|\partial_\xi^i U(s)\| \le C\cdot\min\left\{\frac{e^{s\sqrt{a}\|\xi\|}-1}{\sqrt{a}\|\xi\|}, s\right\}\|v\|. \tag{2.61}$$

The proof is essentially the same as the estimate on U_1 by the assumption. So we omit it. □

Proof of Corollary 2.5 Since M is negatively curved manifold, $\nabla_y^2\left\{\frac{d(x,y)^2}{2}\right\} \ge I_{T_yM}$ and $\|J(1,0,v)\| \ge \|v\|$. See, for example, Corollary 4.6.1 and Theorem 4.6.1 in [23]. Therefore, $\theta_x(y) \ge 1$. By using these estimates, the proof in Theorem 2.4 works. We omit the details. □

Let $P_{x,y}(M) = C([0,1] \to M \mid \gamma(0) = x, \gamma(1) = y)$ and we denote the pinned Brownian motion measure by $\nu_{x,y}$. On $P_{x,y}(M)$, a Dirichlet form is naturally defined by the H-derivative D on $P_{x,y}(M)$. See [1]. Let $\mathfrak{F}C_b^\infty$ be the set of all smooth cylindrical functions on $P_{x,y}(M)$. The following inequality is called a logarithmic Sobolev inequality(=LSI): There exists $C > 0$ such that for all $F \in \mathfrak{F}C_b^\infty$

$$\int_{P_{x,y}(M)} F^2(\gamma)\log\left(F^2(\gamma)/\|F\|^2_{L^2(\nu_{x,y})}\right)d\nu_{x,y}(\gamma) \le C\int_{P_{x,y}(M)} |DF(\gamma)|^2 d\nu_{x,y}(\gamma). \tag{2.62}$$

When M is a Euclidean space, (2.62) holds with $C = 2$ by Gross' result [17]. Driver and Lohrenz [8] proved LSI on loop group for the heat kernel measure which is equivalent to the pinned Brownian motion measure [3, 9]. On the other hand, Eberle [10] proved that

Poincaré's inequality does not hold on a loop space with pinned measure over certain simply connected compact Riemannian manifold. Therefore, LSI does not hold in such a case. But the validity of LSI for pinned measure is still an open problem generally. In the case of Riemannian manifolds with poles, we can prove the following.

THEOREM 2.6. (1) *Assume that* (2.27), (2.29) *with* $\delta < 1/3$ *and* (2.35) *hold. Then* (2.62) *holds in the case where* $x = o$ *and for all* y. *The constant* C *depends only on* a *and* δ.
(2) *Assume* (2.37), (2.39), (2.41) *and* (2.44). *Then* (2.62) *holds for any* x *and* y.

Proof. This follows from Theorem 3.6 in [1] immediately. □

3. Rotationally symmetric case

In this section, we consider rotationally symmetric Riemannian manifolds. We fix an orthonormal frame $\{e_i\}_{i=1}^d \subset T_oM$ and identify T_oM with $\mathbb{R}^d$. Let $\Phi : \mathbb{R}^+ \times S^d \to T_oM$ be the natural map, $\Phi(r, \omega) = r\omega$, where $r = d(o, x), x = \exp(r\omega)$, $(r \geq 0, \omega \in S^{d-1})$, S^{d-1} is the unit sphere centered at the origin in T_oM. g is called a rotationally symmetric if the pull back of g by Φ can be expressed as

$$(\Phi \cdot \exp)^* g = dr^2 + f(r)^2 d\omega^2, \tag{3.1}$$

$d\omega^2$ denotes the standard Riemannian metric on the sphere. We introduce $\varphi(r)$ by $f(r) = re^{\varphi(r)}$. Then by the definition of θ,

LEMMA 3.1.

$$\theta(x) = e^{(d-1)\varphi(r)}. \tag{3.2}$$

Under the assumption of the rotationally symmetry, there exists a smooth function of r, $p(t, r)$ such that $p(t, o, x) = p(t, d(o, x))$. Note that f is a C^∞ function on $[0, \infty)$ satisfying $f(0) = 0$, $f'(0) = 1$ ([19]). Since $f'(0) = 1$, note that $\varphi(0) = 0$. Let $K(r)$ be the radial curvature at x. Then the following Jacobi equation holds (see page 30 in [19]).

$$f''(r) = -K(r)f(r). \tag{3.3}$$

In Section 2, we have given estimates on heat kernels under assumptions on the Riemannian curvature. In this section, we will give similar type estimates on heat kernels in terms of $\varphi(r)$. In rotationally symmetric case, we can go further than general cases. To explain it, let us consider the hyperbolic space with constant negative curvature. In that case, it holds that for any fixed $T > 0$,

$$\sup_{0<t\leq T, x\in M} \left\{ \|\nabla_x \log f(t, x)\|, \|\nabla_x^2 \log f(t, x)\| \right\} < \infty \tag{3.4}$$

where $f(t, x)$ is defined in (2.33) although $\inf_x f(t, x) = 0$ which is excluded under the assumption (2.41). Also $\sup_x \left\| \nabla_x^2 \left\{ \frac{d(o,x)^2}{2} \right\} \right\| = \infty$. In rotationally symmetric case, we can prove (3.4) under an assumption (Assumption 3.2) which is valid for hyperbolic space. Of course, the similar estimate should hold without rotationally symmetry under suitable assumptions. We study this in future papers. We use the following assumption on φ.

ASSUMPTION 3.2. The k-times derivative $\varphi^{(k)}(r)$ is a bounded function on $[0, \infty)$ for all $k \geq 1$. Moreover there exists a C^∞ function ϕ on $[0, \infty)$ such that $\varphi(r) = \phi(r^2)$.

REMARK 3.3. (1) When M is the hyperbolic space with sectional curvature $-a$, then $K(t) \equiv -a$ and $f(r) = \frac{\sinh \sqrt{a} r}{\sqrt{a}}$. Thus

$$\varphi_a(r) = \log \frac{\sinh \sqrt{a} r}{\sqrt{a} r}, \tag{3.5}$$

where we write subscript a to denote the dependence of the curvature. Since the following Taylor expansion holds for all $r \geq 0$,

$$\frac{\sinh \sqrt{ar}}{\sqrt{ar}} = 1 + \sum_{n=1}^{\infty} \frac{(ar)^n}{(2n+1)!},$$

$\varphi_a(\sqrt{r})$ is a smooth function on $[0, \infty)$. Also

$$\varphi_a'(r) = \sqrt{a} \left(\coth(\sqrt{a} r) - \frac{1}{\sqrt{a} r} \right). \tag{3.6}$$

It is easy to see that this function and its all derivatives are bounded functions on $[0, \infty)$. Therefore Assumption 3.2 holds for hyperbolic spaces.

(2) By the Jacobi equation, we have

$$\begin{aligned} K(r) &= -\left(\varphi'(r)^2 + \varphi''(r) + 2\frac{\varphi'(r)}{r} \right), \\ &= -\left(4r^2\phi'(r^2)^2 + 6\phi'(r^2) + 4r^2\phi''(r^2) \right). \end{aligned} \tag{3.7}$$

Therefore, by the lemma below, under Assumption 3.2, it holds that

$$\sup_{r>0} |K(r)| < \infty.$$

LEMMA 3.4. *Under Assumption* 3.2*, for any* $k \geq 1$*,*

$$\sup_{r \geq 0} r^{k/2} |\phi^{(k)}(r)| < \infty. \tag{3.8}$$

Proof. We prove this by induction on k. Because $\varphi(r) = \phi(r^2)$, $\varphi'(r) = 2r\phi'(r^2)$ holds. Since φ' is a bounded function, we have $r^{1/2}\phi'(r)$ is also bounded. We assume that (3.8) holds up to k. Taking $(k+1)$-times derivative, we have

$$\varphi^{(k+1)}(r) = (2r)^{k+1}\phi^{(k+1)}(r^2) + G_k(r).$$

Here $G_k(r)$ is the sum of the function $r^m \phi^{(l)}(r^2)$, where nonnegative integers m and l satisfy that $m < l < k+1$. Hence by the assumption of induction, $G_k(r)$ is a bounded function on $[0, \infty)$. Noting that $\varphi^{(k+1)}$ is also bounded, we see that induction is completed. □

The following follows from a formula in page 30 in [19].

LEMMA 3.5. *Let* F *be a* C^2*-function on* $\mathbb{R}$*. Then we have*

$$\nabla_x^2 F(r) = F'(r) \left(\frac{1}{r} + \varphi'(r) \right) P_x^{\perp} + F''(r) P_x. \quad (r \neq 0), \tag{3.9}$$

where P_x *denotes the projection operator onto the 1-dimensional subspace in* T_xM *spanned by* $v_x \in T_xM$ *where* $\exp_x v_x = o$ *and* $P_x^{\perp}$ *denotes the orthogonal projection.*

When M is rotationally symmetric, Elworthy and Truman's formula reads the following simple one.

Lemma 3.6. *Assume Assumption* 3.2. *Then* V *in Theorem* 2.1 *is given by* $V(x) = \tilde{V}(r^2)$, *where*

$$\tilde{V}(z^2) \quad = \quad -\frac{d-1}{4}\left(\varphi''(z) + (d-1)\frac{\varphi'(z)}{z} + \frac{d-1}{2}\varphi'(z)^2\right). \tag{3.10}$$

Consequently, we have the following representation of $h(t,r) = h(t,o,x)$ *using the pinned standard Brownian motion* $\{W_s\}_{0\le s\le t}$ *on* $\mathbb{R}^d$ *with* $W_0 = W_t = 0$*:*

$$h(t,r) = E\left[\exp\left(\int_0^t \tilde{V}(|W_s + \frac{t-s}{t}r\eta|^2)ds\right)\right], \tag{3.11}$$

where η *denotes a unit vector in* $\mathbb{R}^d$ *and the expectation is independent of* η. *Moreover,* $\tilde{V}$ *is a smooth function and* $\tilde{V}(z)$, $\tilde{V}'(z)z^{1/2}$, $\tilde{V}''(z)z$ *are bounded functions on* $[0,\infty)$.

Proof. (3.11) follows from Theorem 2.1. Boundedness of $\tilde{V}$ and its derivatives follows from Lemma 3.4. □

Comparing to general cases, we do not encounter with the differentiability problem with respect to the initial point of the solution of SDE and we obtain

Theorem 3.7. *Assume Assumption* 3.2. *We have the following explicit expression and an estimate for the Hessian of the logarithm of the heat kernel.*

$$\begin{aligned}\nabla_x^2 \log p(t,o,x) \quad &= \quad -\frac{1}{t}\left(I + r\varphi'(r)P_x^{\perp}\right) - \left(\frac{d-1}{2}\varphi''(r) - \frac{\partial^2}{\partial r^2}\log h(t,r)\right)P_x \\ &\quad - \left(\frac{1}{r} + \varphi'(r)\right)\left(\frac{d-1}{2}\varphi'(r) - \frac{\partial}{\partial r}\log h(t,r)\right)P_x^{\perp}\end{aligned}$$

and for any $T > 0$,

$$\sup_{x\in M, 0<t\le T}\left\|\nabla_x \log p(t,o,x) - \frac{v_x}{t}\right\| \quad < \quad \infty, \tag{3.12}$$

$$\sup_{x\in M, 0<t\le T}\left\|\nabla_x^2 \log p(t,o,x) + \frac{1}{t}(I + r\varphi'(r)P_x^{\perp})\right\| \quad < \quad \infty, \tag{3.13}$$

where v_x *is defined in Lemma* 3.5 (1). *The estimates in* (3.12) *and* (3.13) *depends only on* φ *and* T.

Proof. This follows from Lemma 3.5 and Lemma 3.6. □

The following theorem also follows from Theorem 3.6 in [1] and Theorem 3.7.

Theorem 3.8. *Assume Assumption* 3.2 *and* $\inf_{r\ge 0} r\varphi'(r) > -\frac{1}{2}$, $\sup_{r\ge 0}|r\varphi'(r)| < \infty$. *Then* (2.62) *holds in the case where* $x = o$ *and any* $y \in M$.

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