

Probability Versions of Li-Yau Type Inequalities and Applications ^{*}

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July 11, 2025

Abstract

By using stochastic analysis, two probability versions of Li-Yau type inequalities are established for diffusion semigroups on a manifold possibly with (non-convex) boundary. The inequalities are explicitly given by the Bakry-Emery curvature-dimension, as well as the lower bound of the second fundamental form if the boundary exists. As applications, a number of global and local estimates are presented, which extend or improve existing ones derived for manifolds without boundary. Compared with the maximum principle technique developed in the literature, the probabilistic argument we used is more straightforward and hence considerably simpler.

AMS subject Classification: 58J65, 60H30.

Keywords: Riemannian manifold, Li-Yau type inequality, dimension-curvature, second fundamental form, [martingale](#).

1 Introduction

Since Li-Yau [?] established their famous parabolic Harnack inequality for the heat semigroup on Riemannian manifolds, a number of extensions and refinements have been intensively made in the literature, which will be briefly recalled latter on.

^{*}Supported in part by the National Key R&D Program of China (No. 2022YFA1006000, 2020YFA0712900), State Key Laboratory of Synthetic Biology in Tianjin University, and NNSFC (??).

The purpose of this paper is to provide probability versions of Li-Yau type inequalities for the diffusion semigroups on a complete Riemannian manifold possibly with a Neumann boundary, which are formulated by expectations on functionals of the corresponding diffusion process, which are explicitly given by the Bakry-Emery curvature-dimension of the generator, the second fundamental form of the boundary if exists, and an adapted process ℓ_s satisfying $\ell_0 = 1$ and $\ell_t = 1$, see Theorem ???. With specific choices of the reference adapted process ℓ_s , these inequalities imply new explicit gradient estimates on the heat semigroup, see Corollary ?? for global estimates and Corollary ?? for local estimates.

Compared with the maximum principle technique developed from [?] and adopted in substantial references, the martingale argument we used here considerably simplify the proof. The main idea of the study comes from Arnaudon-Thalmaier [?], where some global and local gradient estimates on the heat semigroup is presented by using stochastic analysis on manifolds.

Before moving on, let us recall some existing results on Li-Yau type inequalities, which are derived on manifolds without boundary, and in most cases for the Laplacian without drift. See [?, ?] for extensions to manifolds with boundary.

Let M be an m -dimensional connected complete Riemannian manifold without boundary, let $L := \Delta + Z$ for some vector field Z . Assume that for some constants $n \geq m$ and $K \in \mathbb{R}$ the following Bakry-Emery curvature-dimension condition holds:

$$(1.1) \quad \text{Ric}_Z^{(n-m)} := \text{Ric}_Z - \frac{Z \otimes Z}{n-m} \geq K,$$

where $\text{Ric}_Z := \text{Ric} - \nabla Z$ is the Bakry-Emery curvature, and Ric is the Ricci curvature. This condition is equivalent to

$$(1.2) \quad \frac{1}{2}L|\nabla f|^2 - \langle \nabla Lf, \nabla f \rangle \geq K|\nabla f|^2 + \frac{1}{n}(Lf)^2, \quad f \in C^\infty(M).$$

When $Z = 0$ we may take $n = m$ in (??), so that this condition reduces to $\text{Ric} \geq K$.

Consider a bounded positive solution to the heat equation

$$\partial_t u_t = L u_t, \quad t \geq 0.$$

Li-Yau [?] proved that when $Z = 0$ and $\text{Ric} \geq K$ for some constant K ,

$$\frac{|\nabla u_t|^2}{u_t^2} \leq \alpha \frac{\Delta u_t}{u_t} + \frac{nK^- \alpha^2}{2(\alpha-1)} + \frac{n\alpha^2}{2t}, \quad t > 0, \alpha > 1,$$

where $K^- := \max\{-K, 0\}$ is the negative part of K . In particular, when $K = 0$ (i.e. $\text{Ric} \geq 0$) with $\alpha \downarrow 1$, this implies

$$\frac{|\nabla u_t|^2}{u_t^2} \leq \frac{\Delta u_t}{u_t} + \frac{n}{2t},$$

where the equality holds for u_t being the standard heat kernel on $M = \mathbb{R}^n$.

The above Li-Yau inequality has been extensively extended or refined. For instances, by Davies [?] (for $Z = 0$)

$$(1.3) \quad \frac{|\nabla u_t|^2}{u_t^2} \leq \alpha \frac{\Delta u_t}{u_t} + \frac{nK^- \alpha^2}{4(\alpha-1)} + \frac{n\alpha^2}{2t}, \quad \alpha > 1, t > 0;$$

by Yau [?] (for $Z = 0$)

$$\frac{|\nabla u_t|^2}{u_t^2} \leq \frac{\Delta u_t}{u_t} + \sqrt{2nK^-} \sqrt{\frac{|\nabla u_t|^2}{u_t} + \frac{n}{2t} + 2nK^- + \frac{n}{2t}}, \quad t > 0,$$

which is then improved by Bakry-Qian [?, (6)]

$$\frac{|\nabla u_t|^2}{u_t^2} \leq \frac{\Delta u_t}{u_t} + \sqrt{nK^-} \sqrt{\frac{|\nabla u_t|^2}{u_t^2} + \frac{n}{2t} + \frac{nK^-}{4} + \frac{n}{2t}},$$

by [?, (54)]

$$(1.4) \quad \frac{|\nabla u_t|^2}{u_t^2} \leq \left(1 + \frac{2}{3}K^-t\right) \frac{\Delta u_t}{u_t} + \frac{n}{2t} + \frac{nK^-}{2} \left(1 + \frac{1}{3}K^-t\right), \quad t > 0;$$

and more recently by Bakry-Bolley-Gentil [?] (also for $Z \neq 0$)

$$(1.5) \quad \frac{4}{nK} \frac{Lu_t}{u_t} < 1 + \frac{\pi^2}{K^2 t^2},$$

$$(1.6) \quad \frac{|\nabla u_t|^2}{u_t^2} \leq \frac{Lu_t}{u_t} - \frac{nK}{2} + \frac{n}{2} \Phi_t \left(1 - \frac{4}{nK} \frac{Lu_t}{u_t}\right), \quad t > 0,$$

where

$$\Phi_t(r) := \begin{cases} K\sqrt{r} \coth(Kt\sqrt{r}), & r > 0, \\ \frac{1}{t}, & r = 0, \\ K\sqrt{-r} \cot(Kt\sqrt{-r}), & -\frac{\pi^2}{K^2 t^2} < r < 0. \end{cases}$$

Moreover, Li-Xu [?] proved (for $Z = 0$)

$$(1.7) \quad \frac{|\nabla u_t|^2}{u_t^2} \leq \left(1 + \frac{\sinh(K^-t) \cosh(K^-t) - K^-t}{\sinh^2(K^-t)}\right) \frac{\Delta u_t}{u_t} + \frac{nK^-}{2} \left(1 + \coth(K^-t)\right), \quad t > 0,$$

see also Qian [?, ?] for conditions on functions a and c such that

$$\frac{|\nabla u_t|^2}{u_t^2} \leq a(t) \frac{\Delta u_t}{u_t} + c(t), \quad t > 0.$$

All these inequalities are proved by using the technique of maximum principle developed in Li-Yau [?].

In the next section, we present two probability versions of Li-Yau type inequalities for the heat semigroup generated by $L := \Delta + Z$ with Neumann boundary if ∂M is non-empty, by using the diffusion process X_t generated by L with reflecting boundary if ∂M is non-empty. The inequalities are explicitly given by K and n in (??) for some constant $n \geq m$ and a function $K \in C(M)$, and the lower bound of the second fundamental form of ∂M if it exists. As applications, besides extensions of existing estimates to the case with boundary, some new global and local estimates are presented in Sections 3 and 4 respectively, where the curvature may be unbounded from below.

2 General results

Let M be an m -dimensional connected complete Riemannian manifold possibly with a boundary ∂M . Let $L := \Delta + Z$ for some vector field Z such that (??) holds for some constant $n \geq m$ and a function $K \in C(M)$. When ∂M exists, let $\sigma \in C(\partial M)$ be a lower bound of the second fundamental form of ∂M , i.e. the inward unit normal vector field N of ∂M satisfies

$$(2.1) \quad \mathbb{I}(v, v) := -\langle \nabla_v N, v \rangle \geq \sigma|v|^2, \quad v \in T\partial M.$$

From now on, let $0 \leq u_0 \in \mathcal{D}(L) \cap C_b^2(M)$ be positive with bounded $u_0 + |Lu_0|$, and $Nu_0|_{\partial M} = 0$ if ∂M exists. Let $u : [0, \infty) \times M \rightarrow (0, \infty)$ solve the following heat equation

$$(2.2) \quad \partial_t u_t(x) = Lu_t(x), \quad Nu_t|_{\partial M} = 0, \quad t \geq 0, \quad x \in M,$$

where the Neumann boundary condition $Nu_t|_{\partial M} = 0$ applies only when ∂M exists.

Let X_t be the diffusion process generated by L with reflecting boundary if ∂M exists, which can be constructed as the unique solution to the following SDE on M :

$$(2.3) \quad dX_t = Z(X_t)dt + \sqrt{2}U_t \circ dB_t + N(X_t)d\mathcal{L}_t,$$

where B_t is the standard m -dimensional Brownian motion on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with natural filtration $\{\mathcal{F}_t\}_{t \geq 0}$, U_t is the horizontal lift of X_t to the frame bundle $O(M)$, and \mathcal{L}_t is the local time of X_t on ∂M if exists, so that $\mathcal{L}_t = 0$ if ∂M does not exist. For any $x \in M$ let \mathbb{E}^x denote the expectation taken for the diffusion process with initial value $X_0 = x$. By (??) and Itô's formula, we have

$$(2.4) \quad u_t(x) = \mathbb{E}^x[u_0(X_t)], \quad Lu_t(x) = \mathbb{E}^x[Lu_0(X_t)], \quad t \geq 0, \quad x \in M.$$

In the following two subsections, we present a global probability version and a local probability version of Li-Yau type inequalities for u_t respectively.

When ∂M is either empty or convex (i.e. $\sigma = 0$) so that $\sigma(X_s)d\mathcal{L}_s = 0$, and K is a constant, by choosing deterministic ℓ_s with $\ell_0 = 1$ and $\ell_t = 0$, and applying the equations in (??), the estimate (??) below reduces to

$$(2.5) \quad \frac{|\nabla u_t|^2}{u_t^2} \leq \frac{n}{2} \int_0^t |\ell'_s|^2 e^{-2Ks} ds - \frac{Lu_t}{u_t} \int_0^t (\ell_s^2)' e^{-2Ks} ds, \quad t > 0,$$

which has been proved in [?, Proposition 2.4] (see also [?]) by using analytic arguments.

Theorem 2.1. *Assume (??) for some constant $n \geq m$ and a function $K \in C(M)$, and also (??) for some $\sigma \in C(\partial M)$ if ∂M exists. Let $t > 0, x \in M$, and $(\ell_s)_{s \in [0, t]}$ be an adapted real process such that $\ell_0 = 1, \ell_t = 0, \ell'_s$ exists $ds \times \mathbb{P}$ -a.e. on $[0, t] \times \Omega$, and*

$$(2.6) \quad \begin{aligned} & \mathbb{E}^x \left[\sup_{s \in [0, t]} \left(\ell_s^2 e^{\int_0^s [K(X_r)^- dr + \sigma(X_r)^- d\mathcal{L}_r]} \frac{|\nabla u_{t-s}|^2}{u_{t-s}}(X_s) \right) \right] \\ & + \mathbb{E}^x \left[\int_0^t (|\ell'_s|^2 + \ell_s^2) e^{-2 \int_0^s [K(X_r)^- dr + \sigma(X_r)^- d\mathcal{L}_r]} ds \right] < \infty. \end{aligned}$$

Then

(1)

$$(2.7) \quad \begin{aligned} \frac{|\nabla u_t|^2}{u_t}(x) &\leq \frac{n}{2} \mathbb{E}^x \left[u_0(X_t) \int_0^t |\ell'_s|^2 e^{-2 \int_0^s \{K(X_r) dr + \sigma(X_r) d\mathcal{L}_r\}} ds \right] \\ &\quad - \mathbb{E}^x \left[(Lu_0)(X_t) \int_0^t (\ell_s^2)' e^{-2 \int_0^s \{K(X_r) dr + \sigma(X_r) d\mathcal{L}_r\}} ds \right]; \end{aligned}$$

(2) Moreover, if ℓ_s is deterministic with $\ell'_s \leq 0$ and $\sigma = 0$ (i.e. ∂M is convex or empty), then for any $\alpha \in (1, \infty)$ and any constant K_0 such that $K \geq K_0$,

$$(2.8) \quad \begin{aligned} (1 + \gamma_{t,\alpha}) \frac{|\nabla u_t|^2}{u_t}(x) - Lu_t(x) \\ \leq \frac{n\alpha}{2} \mathbb{E}^x \left[u_0(X_t) \int_0^t \left(\frac{K(X_s)}{\alpha-1} \ell_s + \ell'_s \right)^2 e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} ds \right], \end{aligned}$$

where

$$\gamma_{t,\alpha} := 2K_0 \int_0^t \ell_s^2 e^{\frac{2\alpha}{\alpha-1} K_0 s} ds > \frac{1}{\alpha} - 1.$$

Proof. (a) When ∂M is non-empty, noting that $Nu_s|_{\partial M} = 0$ implies $\nabla u_s|_{\partial M} \in T\partial M$, we derive from (??) that on ∂M ,

$$(2.9) \quad N \frac{|\nabla u_s|^2}{u_s} = \frac{N|\nabla u_s|^2}{u_s} = \frac{2\mathbb{I}(\nabla u_s, \nabla u_s)}{u_s} \geq 2\sigma(X_s) \frac{|\nabla u_s|^2}{u_s}, \quad s > 0.$$

Next, u is the solution to the equation (??) which implies

$$(2.10) \quad (L + \partial_s)u_{t-s} = 0 = (L + \partial_s)Lu_{t-s}, \quad s \in [0, t).$$

This together with the Bochner-Weitzenböck formula leads to

$$\begin{aligned} (L + \partial_s) \left(\frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right) &= \frac{1}{u_{t-s}} (L|\nabla u_{t-s}|^2 - 2\langle \nabla Lu_{t-s}, \nabla u_{t-s} \rangle) \\ &\quad - \frac{4}{u_{t-s}^2} \text{Hess}_{u_{t-s}}(\nabla u_{t-s}, \nabla u_{t-s}) + \frac{2|\nabla u_{t-s}|^4}{u_{t-s}^3} \\ &= \frac{2}{u_{t-s}} \left(\|\text{Hess}_{u_{t-s}}\|_{HS}^2 - \frac{2}{u_{t-s}} \text{Hess}_{u_{t-s}}(\nabla u_{t-s}, \nabla u_{t-s}) + \frac{|\nabla u_{t-s}|^4}{u_{t-s}^2} + \text{Ric}_Z(\nabla u_{t-s}, \nabla u_{t-s}) \right) \\ &= \frac{2}{u_{t-s}} \left\| \text{Hess}_{u_{t-s}} - \frac{\nabla u_{t-s} \otimes \nabla u_{t-s}}{u_{t-s}} \right\|_{HS}^2 + \frac{2}{u_{t-s}} \text{Ric}_Z(\nabla u_{t-s}, \nabla u_{t-s}) \\ &\geq \frac{2}{mu_{t-s}} \left(\Delta u_{t-s} - \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right)^2 + \frac{2}{u_{t-s}} \text{Ric}_Z(\nabla u_{t-s}, \nabla u_{t-s}). \end{aligned}$$

Combining this with (??) and the fact that

$$\frac{1}{m} \left(\Delta u_{t-s} - \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right)^2 = \frac{1}{m} \left(Lu_{t-s} - \frac{|\nabla u_{t-s}|^2}{u_{t-s}} - Zu_{t-s} \right)^2$$

$$\geq \frac{1}{n} \left(L u_{t-s} - \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right)^2 - \frac{|Z u_{t-s}|^2}{n-m},$$

we derive

$$(2.11) \quad (L + \partial_s) \left(\frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right) \geq \frac{2}{n u_{t-s}} \left(L u_{t-s} - \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right)^2 + 2K \frac{|\nabla u_{t-s}|^2}{u_{t-s}}, \quad s \in [0, t].$$

In the following, we use the above estimates and Itô's formula to prove (??) and (??) respectively. For simplicity, let \geq^m , \leq^m and \equiv^m denote the corresponding inequalities and equality up to an additive local martingale term.

(b) Let $h_s = \ell_s^2$. By (??), (??), (??) and Itô's formula, we obtain

$$\begin{aligned} & d \left(h_s e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} \frac{|\nabla u_{t-s}|^2}{u_{t-s}}(X_s) \right) \\ & \stackrel{m}{=} e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} \left\{ (h'_s - 2h_s K(X_s)) \frac{|\nabla u_{t-s}|^2}{u_{t-s}}(X_s) + h_s \left[(L + \partial_s) \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right](X_s) \right\} ds \\ & \quad + h_s e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} \left(N \left(\frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right) - 2\sigma \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right)(X_s) d\mathcal{L}_s \\ & \geq h'_s e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} \left(\frac{|\nabla u_{t-s}|^2}{u_{t-s}} - L u_{t-s} + L u_{t-s} \right)(X_s) ds \\ & \quad + \frac{2h_s}{n u_{t-s}(X_s)} e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} \left(L u_{t-s} - \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right)^2(X_s) ds \\ & \geq - \frac{n|h'_s|^2}{8h_s} e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} u_{t-s}(X_s) ds + h'_s e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} L u_{t-s}(X_s) ds. \end{aligned}$$

Since $h_s = \ell_s^2$, $h_0 = 1$ and $h_t = 0$, and $|u| + |Lu|$ is bounded on $[0, t] \times M$, by (??) and the dominated convergence theorem, this implies

$$(2.12) \quad \begin{aligned} \frac{|\nabla u_t|^2}{u_t}(x) & \leq \frac{n}{2} \mathbb{E}^x \left[\int_0^t u_{t-s}(X_s) |\ell'_s|^2 e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} ds \right] \\ & \quad - \mathbb{E}^x \left[\int_0^t (L u_{t-s})(X_s) (\ell_s^2)' e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} ds \right]. \end{aligned}$$

Noting that (??) and the Markov property imply

$$(2.13) \quad (L u_{t-s})(X_s) = \mathbb{E}^x(L u_0(X_t) | \mathcal{F}_s), \quad u_{t-s}(X_s) = \mathbb{E}^x(u_0(X_t) | \mathcal{F}_s),$$

we derive (??).

(c) Let $\sigma = 0$ and ℓ_s be deterministic with $\ell'_s \leq 0$. Noting that $N L u_{t-s}|_{\partial M} = 0$ for $s \in [0, t]$, by (??), (??) for $\sigma = 0$, and Itô's formula, we obtain

$$d \left(e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \ell_s^2 \left(\frac{|\nabla u_{t-s}|^2}{u_{t-s}} - \alpha L u_{t-s} \right)(X_s) \right)$$

$$\begin{aligned}
&\stackrel{m}{\geq} e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \left(\frac{2K(X_s)}{\alpha-1} \ell_s^2 + 2\ell_s \ell'_s \right) \left(\frac{|\nabla u_{t-s}|^2}{u_{t-s}} - \alpha L u_{t-s} \right) (X_s) ds \\
(2.14) \quad &+ e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \ell_s^2 \left[(L + \partial_s) \left(\frac{|\nabla u_{t-s}|^2}{u_{t-s}} - \alpha L u_{t-s} \right) \right] (X_s) ds, \quad s \in [0, t].
\end{aligned}$$

Combining this with (??) and (??), we obtain

$$\begin{aligned}
&d \left(e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \ell_s^2 \left(\frac{|\nabla u_{t-s}|^2}{u_{t-s}} - \alpha L u_{t-s} \right) (X_s) \right) \\
&\stackrel{m}{\geq} 2\alpha e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \left(\frac{K(X_s)}{\alpha-1} \ell_s^2 + \ell'_s \ell_s \right) \left(\frac{|\nabla u_{t-s}|^2}{u_{t-s}} - L u_{t-s} \right) (X_s) ds \\
&+ \frac{2e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \ell_s^2}{nu_{t-s}(X_s)} \left(L u_{t-s} - \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right)^2 (X_s) ds \\
&- 2(\alpha-1) e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \ell_s \ell'_s \frac{|\nabla u_{t-s}|^2}{u_{t-s}} (X_s) ds \\
&\geq -\frac{n\alpha^2}{2} e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \left(\frac{K(X_s)}{\alpha-1} \ell_s + \ell'_s \right)^2 u_{t-s}(X_s) ds \\
&- 2(\alpha-1) e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \ell_s \ell'_s \frac{|\nabla u_{t-s}|^2}{u_{t-s}} (X_s) ds, \quad s \in [0, t].
\end{aligned}$$

Combining the condition (??) with the boundedness of u and Lu , $\ell_0 = 1$ and $\ell_t = 0$, this implies

$$(2.15) \quad \frac{|\nabla u_t|^2}{u_t}(x) - \alpha L u_t(x) \leq \frac{n\alpha^2}{2} I_1 + (\alpha-1) I_2,$$

where by (??),

$$\begin{aligned}
I_1 &:= \mathbb{E}^x \left[\int_0^t e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \left(\frac{K(X_s)}{\alpha-1} \ell_s + \ell'_s \right)^2 u_{t-s}(X_s) ds \right] \\
&= \mathbb{E}^x \left[u_0(X_t) \int_0^t e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \left(\frac{K(X_s)}{\alpha-1} \ell_s + \ell'_s \right)^2 ds \right],
\end{aligned}$$

and

$$I_2 := 2\mathbb{E}^x \left[\int_0^t e^{\frac{2}{\alpha-1} \int_0^s K(X_r) dr} \ell_s \ell'_s \frac{|\nabla u_{t-s}|^2}{u_{t-s}} (X_s) ds \right].$$

So, to prove (??), it remains to estimate I_2 .

By (??), (??), (??) and Itô's formula, we obtain

$$d \left(e^{-2K_0 s} \frac{|\nabla u_{t-s}|^2}{u_{t-s}} (X_s) \right) \stackrel{m}{\geq} 0, \quad s \in [0, t],$$

which together with $\frac{2}{\alpha-1} K_0 + 2K_0 = \frac{2\alpha}{\alpha-1} K_0$ and $\ell'_s \leq 0$ yields

$$(2.16) \quad I_2 \leq \frac{|\nabla u_t|^2}{u_t}(x) \int_0^t (\ell_s^2)' e^{\frac{2\alpha}{\alpha-1} K_0 s} ds.$$

By $\ell'_s \leq 0, \ell_0 = 1, \ell_t = 0$ and integration by parts formula, we derive

$$(2.17) \quad 0 < - \int_0^t e^{\frac{2\alpha}{\alpha-1} K_0 s} (\ell_s^2)' ds = 1 + \frac{2\alpha}{\alpha-1} \int_0^t \ell_s^2 K_0 e^{\frac{2\alpha}{\alpha-1} K_0 s} ds = 1 + \frac{\alpha}{\alpha-1} \gamma_{t,\alpha}.$$

So, $\gamma_{t,\alpha} > \frac{1}{\alpha} - 1$ and combining with (??) and (??) implies (??). \square

Remark 2.2. By using $u_0 + \varepsilon$ replacing u_0 then letting $\varepsilon \rightarrow 0$, we may and do assume that $\inf u_0 > 0$. When M is compact, the continuous functions $\frac{|\nabla u|^2}{u}$ on $[0, T] \times M$ as well as K and σ on M are bounded, so that the condition (??) is easily checked. When M is non-compact, if one of the following two conditions hold:

1) ∂M is either convex or empty;

2) \mathbb{I} and Z are bounded, the sectional curvature on M is bounded above, and $K \in C_b(M)$, then by [?, Theorem 3.2.9], see also [?] for $Z = 0$ and M is compact, we have

$$(2.18) \quad |\nabla u_t(x)| \leq \mathbb{E}^x \left[|\nabla u_0|(X_t) e^{-\int_0^t \{K(X_s)ds + \sigma(X_s)d\mathcal{L}_s\}} \right], \quad t > 0.$$

Moreover, $\mathbb{E} e^{p\mathcal{L}_t} < \infty$ holds for any constants $t, p > 0$. Hence, the boundedness of $|\nabla u_0|$ implies that of $|\nabla u|$ on $[0, T] \times M$, and (??) holds provided K is bounded from below and there exists a constant $\delta > 2$ such that

$$(2.19) \quad \mathbb{E}^x \int_0^t |\ell'_s|^\delta ds < \infty,$$

since $|\ell_s| = |\int_s^t \ell'_s ds| \leq (\int_0^t |\ell'_s|^\delta ds)^{\frac{1}{\delta}}$.

When ∂M is non-convex, to apply Theorem ?? we have to estimate the exponential moment of the local time, which have been done in [?, ?, ?]. However, in this way one can only derive a weaker version of Li-Yau inequality where in the upper bound u_t and Lu_t are enlarged as $(P_t u_0^p)^{\frac{1}{p}}$ and $(P_t |Lu_0|^p)^{\frac{1}{p}}$ for some constant $p > 1$.

To derive the exact Li-Yau type inequality for non-convex M , we present the following result by modifying the proof of Theorem ??.. To this end, we follow the line of [?] to make use of a reference function in the following class:

$$\mathcal{D} := \{1 \leq \phi \in C_b^2(M) : (\mathbb{I} + N \log \phi)|_{\partial M} \geq 0\}.$$

Concrete choices of $\phi \in \mathcal{D}$ can be found in [?] as functions of the distance to ∂M , which are explicitly constructed by using bounds on the sectional curvature of M and the second fundamental form of ∂M , see also the proof of Corollary ?? below.

Theorem 2.3. Let ∂M be non-convex, and let (??) hold for some $K \in C_b(M)$. Assume that there exists $\phi \in \mathcal{D}$ such that $\|Z\phi\|_\infty < \infty$. Then

$$(2.20) \quad \begin{aligned} K_\phi &:= 2 \inf_M \{K + \phi^{-1} L\phi\} > -\infty, \\ K_{\alpha,\phi} &:= 2 \inf_M \frac{K\phi^2 + \phi L\phi}{\alpha - \phi^2} > -\infty, \quad \alpha > \|\phi\|_\infty^2, \end{aligned}$$

and the following assertions hold for any $t > 0$ and $\ell \in C_b^1([0, t])$ with $\ell_0 = 1$ and $\ell_t = 0$.

(1) For any constant $\varepsilon > 0$,

$$(2.21) \quad \begin{aligned} \frac{\phi^2 |\nabla u_t|^2}{\|\phi\|_\infty^2 u_t^2} &\leq \left(2 \int_0^t \ell_s |\ell'_s| e^{(\varepsilon - K_\phi)s} ds \right) \frac{Lu_t}{u_t} \\ &\quad + \left(\frac{n}{2} + \frac{\|\nabla \log \phi\|_\infty^2}{\varepsilon} \right) \int_0^t (\ell'_s)^2 e^{(\varepsilon - K_\phi)s} ds. \end{aligned}$$

(2) For any constants $\alpha > \|\phi\|_\infty^2$ and $\varepsilon > 0$,

$$(2.22) \quad \begin{aligned} (1 + \gamma_{t,\alpha,\phi}) \frac{\phi^2 |\nabla u_t|^2}{u_t^2} - \alpha \frac{Lu_t}{u_t} \\ \leq \int_0^t e^{(K_{\alpha,\phi} - \varepsilon)s} ((K_{\alpha,\phi} - \varepsilon)\ell_s + 2\ell'_s)^2 \left(\frac{n\alpha^2}{8} + \frac{\alpha^2 \|\nabla \log \phi\|_\infty^2}{4\varepsilon(\alpha - \|\phi\|_\infty^2)} \right) ds, \end{aligned}$$

where $\gamma_{t,\alpha,\phi} = 2 \left(\frac{\alpha}{\|\phi\|_\infty^2} - 1 \right) \int_0^t |\ell_s \ell'_s| e^{(K_{\alpha,\phi} + K_\phi - \varepsilon)s} ds > 0$.

Proof. We may assume that $\inf u_0 > 0$. Since $\phi \in C_b^2(M)$, $\|Z\phi\|_\infty < \infty$ implies condition (3.2.15) in [?], then [?, Theorem 3.2.7] for $f = u_0$ implies the boundedness of $|\nabla u|$ on $[0, t] \times M$. So, $\frac{|\nabla u|^2}{u}$ is bounded on $[0, t] \times M$.

By $\phi \in \mathcal{D}$ and (??) for $\sigma = -(N \log \phi)$, we obtain

$$(2.23) \quad N \left(\frac{\phi^2 |\nabla u_s|^2}{u_s} \right) \Big|_{\partial M} = \frac{2\phi^2}{u_s} (\mathbb{I}(\nabla u_s, \nabla u_s) + (N \log \phi) |\nabla u_s|^2) \Big|_{\partial M} \geq 0.$$

By (??) and the display after (??), we obtain

$$\begin{aligned} (L + \partial_s) \frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} &= \frac{2\phi^2}{u_{t-s}} \left(\left\| \text{Hess}_{u_{t-s}} - \nabla u_{t-s} \otimes \nabla \log u_{t-s} \right\|_{HS}^2 + \text{Ric}_Z(\nabla u_{t-s}, \nabla u_{t-s}) \right) \\ &\quad + \frac{(L\phi^2) |\nabla u_{t-s}|^2}{u_{t-s}} + \frac{4\phi^2}{u_{t-s}} \text{Hess}_{u_{t-s}}(\nabla u_{t-s}, \nabla \log \phi) - \frac{2\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} \langle \nabla \log u_{t-s}, \nabla \log \phi \rangle \\ &= \frac{2\phi^2}{u_{t-s}} \left(\left\| \text{Hess}_{u_{t-s}} - \nabla u_{t-s} \otimes \nabla \log \frac{u_{t-s}}{\phi} \right\|_{HS}^2 + \text{Ric}_Z(\nabla u_{t-s}, \nabla u_{t-s}) \right) \\ &\quad + \frac{|\nabla u_{t-s}|^2 (L\phi^2 - 2|\nabla \phi|^2)}{u_{t-s}} \\ &\geq \frac{2\phi^2}{u_{t-s}} \left[\frac{1}{m} \left(Lu_{t-s} - \left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle - Zu_{t-s} \right)^2 + \text{Ric}_Z(\nabla u_{t-s}, \nabla u_{t-s}) \right] \\ &\quad + \frac{2(\phi L\phi) |\nabla u_{t-s}|^2}{u_{t-s}} \\ &\geq \frac{2\phi^2}{u_{t-s}} \left[\frac{1}{n} \left(Lu_{t-s} - \left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle \right)^2 + \text{Ric}_Z^{(n-m)}(\nabla u_{t-s}, \nabla u_{t-s}) \right] \\ &\quad + \frac{2(\phi L\phi) |\nabla u_{t-s}|^2}{u_{t-s}} \\ &\geq \frac{2\phi^2}{nu_{t-s}} \left(Lu_{t-s} - \left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle \right)^2 + \frac{2(K\phi^2 + \phi L\phi) |\nabla u_{t-s}|^2}{u_{t-s}}. \end{aligned}$$

Hence, (??) and (??) yield

$$\begin{aligned}
(2.24) \quad & (L + \partial_s) \frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} \\
& \geq \frac{2\phi^2}{nu_{t-s}} \left(Lu_{t-s} - \left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle \right)^2 + \frac{2(K\phi^2 + \phi L\phi) |\nabla u_{t-s}|^2}{u_{t-s}} \\
& \geq \frac{2\phi^2}{nu_{t-s}} \left(Lu_{t-s} - \left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle \right)^2 + \frac{K_\phi \phi^2 |\nabla u_{t-s}|^2}{u_{t-s}}.
\end{aligned}$$

(a) By (??), (??) and Itô's formula, we derive

$$\begin{aligned}
& d \left(\ell_s^2 e^{(\varepsilon - K_\phi)s} \frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} (X_s) \right) \\
& \stackrel{m}{\geq} 2\ell_s^2 e^{(\varepsilon - K_\phi)s} \frac{\phi^2(X_s)}{nu_{t-s}} \left(Lu_{t-s} - \left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle \right)^2 (X_s) ds \\
& \quad + 2\ell_s \ell'_s e^{(\varepsilon - K_\phi)s} \phi^2(X_s) \left(\left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle - Lu_{t-s} \right) (X_s) ds \\
& \quad + 2\ell_s \ell'_s e^{(\varepsilon - K_\phi)s} \phi^2(X_s) \left(Lu_{t-s} + \langle \nabla u_{t-s}, \nabla \log \phi \rangle \right) (X_s) ds \\
& \quad + \varepsilon \ell_s^2 e^{(\varepsilon - K_\phi)s} \frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} (X_s) ds \\
& \geq e^{(\varepsilon - K_\phi)s} \phi^2(X_s) \left((\ell_s^2)' Lu_{t-s} + 2\ell_s \ell'_s \langle \nabla u_{t-s}, \nabla \log \phi \rangle + \frac{\varepsilon \ell_s^2 |\nabla u_{t-s}|^2}{u_{t-s}} - \frac{n(\ell'_s)^2 u_{t-s}}{2} \right) (X_s) ds.
\end{aligned}$$

Thus,

$$\begin{aligned}
(2.25) \quad & d \left(\ell_s^2 e^{(\varepsilon - K_\phi)s} \frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} (X_s) \right) \\
& \stackrel{m}{\geq} e^{(\varepsilon - K_\phi)s} \phi^2(X_s) \left[(\ell_s^2)' Lu_{t-s} - \left(\frac{n}{2} + \frac{\|\nabla \log \phi\|_\infty^2}{\varepsilon} \right) (\ell'_s)^2 u_{t-s} \right] (X_s) ds.
\end{aligned}$$

Combining this with the boundedness of $\frac{|\nabla u_{t-s}|^2}{u_{t-s}}$ as explained in the beginning of the proof, $\ell_0 = 1$, $\ell_t = 0$, and that u_t and Lu_t are bounded with

$$\mathbb{E}^x u_{t-s}(X_s) = u_t(x), \quad \mathbb{E}^x Lu_{t-s}(X_s) = Lu_t(x),$$

we derive (??).

(b) Simply denote $\beta = K_{\alpha, \phi} - \varepsilon$. Combining (??) with (??), (??), $NLu_{t-s}|_{\partial M} = 0$ and $(L + \partial_s)Lu_{t-s} = 0$ for $s \in [0, 1]$, and applying Itô's formula to (??), we derive

$$\begin{aligned}
& d \left\{ e^{\beta s} \ell_s^2 \left(\frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} - \alpha Lu_{t-s} \right) (X_s) \right\} \\
& \stackrel{m}{=} e^{\beta s} \left\{ \ell_s^2 (L + \partial_s) \frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} + (\beta \ell_s^2 + 2\ell_s \ell'_s) \left(\frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} - \alpha Lu_{t-s} \right) \right\} (X_s) ds
\end{aligned}$$

$$\begin{aligned}
&\geq e^{\beta s} \left\{ \frac{2\ell_s^2 \phi^2}{nu_{t-s}} \left(Lu_{t-s} - \left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle \right)^2 \right. \\
&\quad \left. - \alpha(\beta\ell_s^2 + 2\ell_s\ell'_s) \left(Lu_{t-s} - \left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle \right) - \alpha(\beta\ell_s^2 + 2\ell_s\ell'_s) \left\langle \nabla u_{t-s}, \nabla \log \frac{u_{t-s}}{\phi} \right\rangle \right. \\
&\quad \left. + \left([\beta + 2K + 2\phi^{-1}L\phi] \ell_s^2 + 2\ell_s\ell'_s \right) \frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} \right\} (X_s) \, ds \\
&\geq e^{\beta s} \left\{ - \frac{n\alpha^2(\beta\ell_s + 2\ell'_s)^2}{8\phi^2} u_{t-s} + (2K\phi^2 + \phi L\phi + \beta(\phi^2 - \alpha)) \ell_s^2 \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right. \\
&\quad \left. - 2\ell_s\ell'_s(\alpha - \phi^2) \frac{|\nabla u_{t-s}|^2}{u_{t-s}} - \alpha |\beta\ell_s^2 + 2\ell_s\ell'_s| \|\nabla \log \phi\|_\infty |\nabla u_{t-s}| \right\} (X_s) \, ds.
\end{aligned}$$

Since $\ell_s\ell'_s < 0$, $\alpha > \phi \geq 1$, and $\beta = K_{\alpha,\phi} - \varepsilon$ yields

$$2K\phi^2 + 2\phi L\phi + \beta(\phi^2 - \alpha) \geq (\beta - K_{\alpha,\phi})(\phi^2 - \alpha) \geq (\alpha - \|\phi\|_\infty^2)\varepsilon,$$

this further implies

$$\begin{aligned}
&d \left\{ e^{\beta s} \ell_s^2 \left(\frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} - \alpha Lu_{t-s} \right) (X_s) \right\} \\
&\geq -e^{\beta s} (\beta\ell_s + 2\ell'_s)^2 \left(\frac{n\alpha^2}{8} + \frac{\alpha^2 \|\nabla \log \phi\|_\infty^2}{4(\alpha - \|\phi\|_\infty^2)\varepsilon} \right) u_{t-s} (X_s) \, ds \\
&\quad + 2|\ell_s\ell'_s|(\alpha\phi^{-2} - 1) e^{\beta s} \frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} (X_s) \, ds.
\end{aligned}$$

Combining this with $\mathbb{E}u_{t-s}(X_s) = u_t(x)$ for $X_0 = x$, the boundedness of $\frac{|\nabla u_{t-s}|^2}{u_{t-s}}$, u_{t-s} , Lu_{t-s} as explained in the beginning of the proof, and $\ell_0 = 1$, $\ell_t = 0$, we derive

$$\begin{aligned}
&\frac{\phi^2 |\nabla u_t|^2}{u_t}(x) - \alpha Lu_t(x) \\
(2.26) \quad &\leq u_t(x) \left(\frac{n\alpha^2}{8} + \frac{\alpha^2 \|\nabla \log \phi\|_\infty^2}{4(\alpha - \|\phi\|_\infty^2)\varepsilon} \right) \int_0^t e^{\beta s} (\beta\ell_s + 2\ell'_s)^2 \, ds \\
&\quad - 2 \int_0^t |\ell_s\ell'_s| e^{\beta s} \mathbb{E} \left[(\alpha - \phi^2) \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right] (X_s) \, ds.
\end{aligned}$$

By (??) for $\ell = 1$ and $\varepsilon \downarrow 0$, we have

$$d \left(e^{-K_\phi s} \frac{\phi^2 |\nabla u_{t-s}|^2}{u_{t-s}} (X_s) \right) \geq 0,$$

so that

$$\begin{aligned}
&- 2 \int_0^t |\ell_s\ell'_s| e^{\beta s} \mathbb{E} \left[(\alpha - \phi^2) \frac{|\nabla u_{t-s}|^2}{u_{t-s}} \right] (X_s) \, ds \\
&\leq -2 \int_0^t |\ell_s\ell'_s| (\alpha \|\phi\|_\infty^{-2} - 1) e^{(\beta+K_\phi)s} \mathbb{E} \left[e^{-K_\phi s} \phi^2 \frac{|\nabla u_{t-s}|^2}{u_{t-s}} (X_s) \right] \, ds
\end{aligned}$$

$$\leq -2(\alpha\|\phi\|_\infty^{-2} - 1) \left(\int_0^t |\ell_s \ell'_s| e^{(\beta+K_\phi)s} ds \right) \frac{|\phi \nabla u_t|^2}{u_t}(x).$$

Combining this with (??), $\beta = K_{\alpha,\phi} - \varepsilon$ and the definition of $\gamma_{t,\alpha,\phi}$, we finish the proof of (??). \square

3 Global Li-Yau type estimates

We will present explicit Li-Yau type estimates by using Theorem ?? and Theorem ?? for the convex and non-convex cases respectively.

3.1 ∂M is convex or empty

By Remark ??, (??) holds for all $\ell \in C_b^1([0, t])$ provided K is bounded from below and ∂M is either convex or empty. Therefore, estimates (??) holds for $\sigma = 0$, and (??) holds for $\ell'_s \leq 0$. By taking specific choices of ℓ_s in these estimates, we present explicit Li-Yau type inequalities in the following Corollaries ?? and ??, where

- (??) improves (??) when $t > \frac{\pi}{K}$, and is sharp for small time as shown by [?, Corollary 2.3];
- (??) and (??) are new even for $Z = 0$ and $\partial M = \emptyset$;
- (??) is due to [?] for $\partial M = \emptyset$, which improves a number of classical bounds recalled in the introduction as shown in [?, Section 5].

When ∂M is strictly convex such that σ is a positive constant, $\mathbb{E}^x[e^{-2\sigma\mathcal{L}_s}]$ decays exponentially fast as $s \rightarrow \infty$ according to [?, Lemma 3.1], so that (??) may provide better estimates than those presented in Corollary ??.

Corollary 3.1. *Assume that ∂M is either empty or convex, and let (??) hold for a constant $K \in \mathbb{R}$. Then the inequality (??) holds for $\sigma = 0$, which implies the following estimates.*

(1) *For any $t > 0$,*

$$(3.1) \quad \frac{Lu_t}{u_t} \begin{cases} \leq \frac{n}{4t} \left[(Kt) \wedge \pi + \frac{\pi^2}{(Kt) \wedge \pi} \right], & \text{if } K > 0, \\ \geq -\frac{n}{4t} \left[\pi \vee (-Kt) + \frac{\pi^2}{\pi \vee (-Kt)} \right], & \text{if } K \leq 0. \end{cases}$$

(2) *When $K \neq 0$, for any constant $\alpha \in \mathbb{R}$ such that $\frac{1+\alpha}{Kt} \geq \frac{9\pi^2-64}{9\pi^2}$, let*

$$\beta_{t,\alpha} := \left(\frac{1+\alpha}{Kt} - \frac{9\pi^2-64}{9\pi^2} \right)^{\frac{1}{2}} - \frac{8}{3\pi}.$$

Then

$$(3.2) \quad \frac{|\nabla u_t|^2}{u_t^2} - \frac{\alpha Lu_t}{u_t} \leq \frac{n}{2} \left(\frac{K(\alpha-1)}{2} + \frac{(1+\alpha)\pi^2}{2Kt^2} - \frac{2\pi\beta_{t,\alpha}}{t} - \frac{3\pi^2}{8t} \right).$$

(3) When $K > 0$, for any constant $K' \geq K$ such that $\text{Ric}_Z \geq K'$, we have

$$(3.3) \quad \frac{|\nabla u_t|^2}{u_t^2} \leq \frac{n}{2} \left(\frac{\pi^2 K}{2[1 \wedge (Kt)]^2} - \frac{K}{2} - \frac{3K\pi^2}{8[1 \wedge (Kt)]} \right) e^{-2K'(t-K^{-1})^+}, \quad t > 0.$$

(4) (??) holds.

Proof. When ∂M is empty or convex, we may take $\sigma = 0$ such that for any deterministic ℓ_s with $\ell_0 = 1$ and $\ell_t = 0$,

$$\int_0^t (\ell_s^2)' e^{-2 \int_0^s [K(X_r) dr + \sigma(X_r) d\mathcal{L}_r]} ds = -1 + 2 \int_0^t K(X_s) e^{-2 \int_0^s K(X_r) dr} \ell_s^2 ds.$$

When K is a constant, then (??) reduces to

$$(3.4) \quad \frac{|\nabla u_t|^2}{u_t^2} \leq \frac{n}{2} \left[\int_0^t |\ell_s'|^2 e^{-2Ks} ds \right] + \left(1 - 2K \int_0^t \ell_s^2 e^{-2Ks} ds \right) \frac{Lu_t}{u_t}.$$

(1) For a fixed constant $a \in \mathbb{R}$, let

$$\ell_s := e^{Ks} \left(\cos \frac{\pi s}{2t} + a \sin \frac{\pi s}{t} \right), \quad s \in [0, t].$$

We have

$$(3.5) \quad \int_0^t \ell_s^2 e^{-2Ks} ds = \int_0^t \left[\cos^2 \frac{\pi s}{2t} + a^2 \sin^2 \frac{\pi s}{t} + 2a \left(\cos \frac{\pi s}{2t} \right) \sin \frac{\pi s}{t} \right] ds,$$

$$(3.6) \quad \begin{aligned} \int_0^t |\ell_s'|^2 e^{-2Ks} ds &= K^2 \int_0^t \ell_s^2 e^{-2Ks} ds - K \\ &+ \int_0^t \left[\frac{\pi^2 a^2}{t^2} \cos^2 \frac{\pi s}{t} + \frac{\pi^2}{4t^2} \sin^2 \frac{\pi s}{2t} - \frac{\pi^2 a}{t^2} \left(\cos \frac{\pi s}{t} \right) \sin \frac{\pi s}{2t} \right] ds. \end{aligned}$$

Note that

$$\begin{aligned} \int_0^t \sin^2 \frac{\pi s}{t} ds &= \frac{t}{\pi} \int_0^\pi \sin^2 \theta d\theta = \frac{t}{2} = \int_0^t \cos^2 \frac{\pi s}{t} ds, \\ \int_0^t \cos^2 \frac{\pi s}{2t} ds &= \frac{2t}{\pi} \int_0^{\frac{\pi}{2}} \cos^2 \theta d\theta = \frac{t}{2} = \int_0^t \sin^2 \frac{\pi s}{2t} ds, \\ \int_0^t \left(\cos \frac{\pi s}{2t} \right) \sin \frac{\pi s}{t} ds &= \frac{2t}{\pi} \int_0^{\frac{\pi}{2}} (\cos \theta) \sin(2\theta) d\theta = -\frac{4t}{\pi} \int_0^{\frac{\pi}{2}} (\cos^2 \theta) d\cos \theta = \frac{4t}{3\pi}, \\ \int_0^t \left(\cos \frac{\pi s}{t} \right) \sin \frac{\pi s}{2t} ds &= \frac{2t}{\pi} \int_0^{\frac{\pi}{2}} (\cos(2\theta)) \sin \theta d\theta = -\frac{2t}{\pi} \int_0^{\frac{\pi}{2}} (2\cos^2 \theta - 1) d\cos \theta = -\frac{2t}{3\pi}. \end{aligned}$$

Combining these with (??) and (??), we obtain

$$(3.7) \quad \begin{aligned} 2K \int_0^t \ell_s^2 e^{-2Ks} ds &= Kt(1 + a^2) + \frac{16Kta}{3\pi}, \\ \int_0^t |\ell_s'|^2 e^{-2Ks} ds &= \frac{K}{2} \left(Kt(1 + a^2) + \frac{16Kta}{3\pi} \right) - K + \frac{\pi^2 a^2}{2t} + \frac{\pi^2}{8t} + \frac{2\pi a}{3t}. \end{aligned}$$

Substituting into (??) and letting $a \rightarrow \infty$, we derive that when $K > 0$,

$$\frac{Lu_t}{u_t} \leq \frac{n}{2} \lim_{a \rightarrow \infty} \frac{\int_0^t |\ell'_s|^2 e^{-2Ks} ds}{2K \int_0^t \ell_s^2 e^{-2Ks} ds} = \frac{n}{4} \left(K + \frac{\pi^2}{Kt^2} \right),$$

while for $K < 0$,

$$\frac{Lu_t}{u_t} \geq \frac{n}{2} \lim_{a \rightarrow \infty} \frac{-\int_0^t |\ell'_s|^2 e^{-2Ks} ds}{-2K \int_0^t \ell_s^2 e^{-2Ks} ds} = \frac{n}{4} \left(K + \frac{\pi^2}{Kt^2} \right).$$

Condition (??) is trivially also satisfied for any $k \leq K$, the derived estimates hence hold for k replacing K as well. By taking $k = K \wedge \frac{\pi}{t}$ for $K > 0$, and $K = K \wedge (-\frac{\pi}{t})$ for $K < 0$, the above estimates for k replacing K imply (??).

(2) By the definition of $\beta_{t,\alpha}$ and (??), we obtain

$$\beta_{t,\alpha}^2 = \frac{1+\alpha}{Kt} - 1 - \frac{16\beta_{t,\alpha}}{3\pi},$$

and

$$2K \int_0^t \ell_s^2 e^{-2Ks} ds = Kt(1 + \beta_{t,\alpha}^2) + \frac{16Kt\beta_{t,\alpha}}{3\pi} = 1 + \alpha.$$

Combining these with (??) and (??) for $a = \beta_{t,\alpha}$, we derive

$$\begin{aligned} \frac{|\nabla u_t|^2}{u_t^2} - \frac{\alpha Lu_t}{u_t} &\leq \frac{n}{2} \int_0^t |\ell'_s|^2 e^{-2Ks} ds \\ &= \frac{n}{2} \left(\frac{(1+\alpha)K}{2} - K + \frac{\pi^2}{2t} \left(\frac{1+\alpha}{Kt} - 1 - \frac{16\beta_{t,\alpha}}{3\pi} \right) + \frac{\pi^2}{8t} + \frac{2\pi\beta_{t,\alpha}}{3t} \right) \\ &\leq \frac{n}{2} \left(\frac{(\alpha-1)K}{2} + \frac{\pi^2(1+\alpha)}{2Kt^2} - \frac{2\pi\beta_{t,\alpha}}{t} - \frac{3\pi^2}{8t} \right). \end{aligned}$$

Then (??) holds.

(3) When $t \leq \frac{1}{K}$ and $\alpha = 0$, we have $\beta_{t,\alpha} \geq 0$, so that (??) implies

$$\begin{aligned} \frac{|\nabla u_t|^2}{u_t^2} &\leq \frac{n}{2} \left(\frac{(\alpha-1)K}{2} + \frac{\pi^2}{2Kt^2} - \frac{2\pi\beta_{t,\alpha}}{t} - \frac{3\pi^2}{8t} \right) \\ (3.8) \quad &\leq \frac{n}{2} \left(\frac{\pi^2}{2Kt^2} - \frac{K}{2} - \frac{3\pi^2}{8t} \right). \end{aligned}$$

Let P_t be the (Neumann) semigroup generated by L . Then $u_t = P_{(t-K^{-1})+} u_{t \wedge K^{-1}}$ and it is well known that $\text{Ric}_Z \geq K'$ implies

$$|\nabla u_t| = |\nabla P_{(t-K^{-1})+} u_{t \wedge K^{-1}}| \leq e^{-K'(t-K^{-1})^+} P_{(t-K^{-1})+} |\nabla u_{t \wedge K^{-1}}|.$$

Combining this with (??) for $t \wedge K^{-1}$ replacing t , we derive (??).

(4) By (??), $\lambda := 1 - \frac{4}{nK} \frac{Lu_t}{u_t} > -\frac{\pi^2}{K^2 t^2}$. Choose $\ell_s = h_s e^{Ks}$ for

$$h_s := \begin{cases} \frac{\sinh(K\sqrt{\lambda}(t-s))}{\sinh(K\sqrt{\lambda}t)}, & \lambda > 0; \\ \frac{t-s}{t}, & \lambda = 0; \\ \frac{\sin(K\sqrt{-\lambda}(t-s))}{\sin(K\sqrt{-\lambda}t)}, & \lambda \in (-\frac{\pi^2}{K^2 t^2}, 0). \end{cases}$$

We have $\ell'_s = h'_s e^{Ks} + K h_s e^{Ks}$. So, (??) implies

$$\begin{aligned}
\frac{|\nabla u_t|^2}{u_t^2} &\leq \frac{n}{2} \int_0^t |\ell'_s|^2 e^{-2Ks} ds - 2 \left[\int_0^t \ell_s \ell'_s e^{-2Ks} ds \right] \frac{Lu_t}{u_t} \\
&= \frac{n}{2} \int_0^t (h'_s + K h_s)^2 ds - \frac{2Lu_t}{u_t} \int_0^t h_s (h'_s + K h_s) ds \\
&= \frac{n}{2} \int_0^t (|h'_s|^2 + 2K h_s h'_s + K^2 h_s^2) ds - \frac{2Lu_t}{u_t} \int_0^t (h_s h'_s + K h_s^2) ds \\
&= \frac{n}{2} \int_0^t |h'_s|^2 ds + \left(Kn - \frac{2Lu_t}{u_t} \right) \int_0^t h_s h'_s ds + \left(\frac{K^2 n}{2} - 2K \frac{Lu_t}{u_t} \right) \int_0^t h_s^2 ds.
\end{aligned}$$

It is easy to see that

$$\int_0^t h_s h'_s ds = \int_0^t h_s dh_s = \frac{h_t^2 - h_0^2}{2} = -\frac{1}{2}.$$

Moreover, by $h''_s = K^2 \lambda h_s$ for $\lambda := 1 - \frac{4}{nK} \frac{Lu_t}{u_t}$ due to the definition of h_s , one has

$$\int_0^t |h'_s|^2 ds = \int_0^t h'_s dh_s = h'_s h_s|_0^t - \int_0^t h''_s h_s ds = -h'_0 - K^2 \left(1 - \frac{4}{nK} \frac{Lu_t}{u_t} \right) \int_0^t h_s^2 ds.$$

We then conclude that

$$\begin{aligned}
\frac{|\nabla u_t|^2}{u_t^2} &\leq \frac{Lu_t}{u_t} - \frac{n}{2} h'_0 - \frac{Kn}{2} - \frac{nK^2}{2} \left(1 - \frac{4}{nK} \frac{Lu_t}{u_t} \right) \int_0^t h_s^2 ds + \left(\frac{K^2 n}{2} - 2K \frac{Lu_t}{u_t} \right) \int_0^t h_s^2 ds \\
&= \frac{Lu_t}{u_t} - \frac{n}{2} h'_0 - \frac{Kn}{2}.
\end{aligned}$$

This implies (??) by noting that $h'_0 = -\Phi_t(\lambda)$. \square

Estimates in the next corollary are implied by (??), where (??) is new, and (??) improves (??) by noting that for $K < 0$ and $\alpha > 1$,

$$\frac{K}{4} \coth \left(\frac{Kt}{2(\alpha-1)} \right) < \frac{K}{2} + \frac{\alpha-1}{2t},$$

and as in (??) we have

$$\frac{2K \int_0^t (1 - e^{-\frac{Ks}{\alpha-1}})^2 ds}{\alpha (1 - e^{-\frac{Kt}{\alpha-1}})^2} > \frac{1}{\alpha} - 1.$$

Corollary 3.2. *Assume that ∂M is either empty or convex, and let (??) hold for a constant $K \in \mathbb{R}$. Then the inequality (??) holds for $\sigma = 0$ and implies the following estimates.*

(1) *For any constant $\alpha > 1$*

$$\begin{aligned}
(3.9) \quad &\left(1 + \frac{2K \int_0^t (1 - e^{-\frac{Ks}{\alpha-1}})^2 e^{2K(t-s)} ds}{(1 - e^{-\frac{Kt}{\alpha-1}})^2} \right) \frac{|\nabla u_t|^2}{u_t^2} \\
&\leq \frac{Lu_t}{u_t} + \frac{nK\alpha}{4(\alpha-1)} \coth \left(\frac{Kt}{2(\alpha-1)} \right), \quad t > 0.
\end{aligned}$$

(2) For any $t > 0$ and $\alpha > 1$,

$$(3.10) \quad \left(\frac{e^{2Kt} - 1}{2K^2 t^2} - \frac{1}{Kt} \right) \frac{|\nabla u_t|^2}{u_t^2} \leq \frac{Lu_t}{u_t} + \frac{n\alpha}{2t}.$$

Consequently, when $K > 0$,

$$(3.11) \quad \left(1 + \frac{2}{3}Kt \right) \frac{|\nabla u_t|^2}{u_t^2} \leq \frac{Lu_t}{u_t} + \frac{n}{2t}, \quad t > 0.$$

Proof. If (??) holds for a constant $K \in \mathbb{R}$ and ∂M is convex or empty, then the inequality (??) reduces to

$$(3.12) \quad (1 + \gamma_{t,\alpha}) \frac{|\nabla u_t|^2}{u_t^2} - \frac{Lu_t}{u_t} \leq \frac{n\alpha}{2} \int_0^t \left(\frac{K}{\alpha-1} \ell_s + \ell'_s \right)^2 e^{\frac{2\alpha}{\alpha-1} Ks} ds,$$

where

$$\gamma_{t,\alpha} := 2K \int_0^t \ell_s^2 e^{\frac{2\alpha}{\alpha-1} Ks} ds > \frac{1}{\alpha} - 1.$$

(1) Let $\ell_s = \frac{\int_0^{t-s} e^{\frac{Kr}{\alpha-1}} dr}{\int_0^t e^{\frac{Kr}{\alpha-1}} dr}$, $s \in [0, t]$. Then $\ell_0 = 1$, $\ell_t = 0$ and

$$\ell'_s = \frac{-e^{\frac{K(t-s)}{\alpha-1}}}{\int_0^t e^{\frac{Kr}{\alpha-1}} dr} = \frac{-K}{\alpha-1} \ell_s - \frac{1}{\int_0^t e^{\frac{Kr}{\alpha-1}} dr} \leq 0.$$

So,

$$\int_0^t e^{\frac{2Ks}{\alpha-1}} \left(\ell'_s + \frac{K}{\alpha-1} \ell_s \right)^2 ds = \frac{\int_0^t e^{\frac{2Ks}{\alpha-1}} ds}{(\int_0^t e^{\frac{Ks}{\alpha-1}} dr)^2} = \frac{K}{2(\alpha-1)} \coth \left(\frac{Kt}{2(\alpha-1)} \right).$$

Moreover, according to the definition of $\gamma_{t,\alpha}$,

$$\gamma_{t,\alpha} = 2K \int_0^t \left(\frac{\int_0^{t-s} e^{\frac{Kr}{\alpha-1}} dr}{\int_0^t e^{\frac{Kr}{\alpha-1}} dr} \right)^2 e^{\frac{2\alpha}{\alpha-1} Ks} ds = \frac{2K \int_0^t (1 - e^{-\frac{Ks}{\alpha-1}})^2 e^{2K(t-s)} ds}{(1 - e^{-\frac{Kt}{\alpha-1}})^2}.$$

Then (??) follows by combining these estimates with (??).

(2) For $\alpha \in (1, \infty)$, let

$$\ell_s = e^{-\frac{Ks}{\alpha-1}} \frac{t-s}{t}, \quad s \in [0, t].$$

Then $\ell_0 = 1$, $\ell_t = 0$, and when $\alpha \geq 1 + K^- t$ we have

$$\begin{aligned} \ell'_s &= -\frac{K}{\alpha-1} \ell_s - \frac{1}{t} e^{-\frac{Ks}{\alpha-1}} \leq 0, \\ \ell'_s + \frac{K}{\alpha-1} \ell_s &= -\frac{1}{t} e^{-\frac{Ks}{\alpha-1}}. \end{aligned}$$

Then

$$\int_0^t e^{\frac{2K}{\alpha-1}s} \left(\frac{K}{\alpha-1} \ell_s + \ell'_s \right)^2 ds = \int_0^t \frac{1}{t^2} ds = \frac{1}{t},$$

$$\gamma_{t,\alpha} = 2K \int_0^t \left(\frac{t-s}{t} \right)^2 e^{2Ks} ds = \frac{e^{2Kt} - 1}{2K^2 t^2} - \frac{1}{Kt} - 1.$$

Thus, (??) implies (??), and further (??) by estimating

$$1 + \gamma_{t,\alpha} = \frac{e^{2Kt} - 1}{2K^2 t^2} - \frac{1}{Kt} \geq 1 + \frac{2}{3} Kt,$$

and letting $\alpha \downarrow 1$ when $K > 0$. □

3.2 ∂M is non-convex

Let ρ_∂ be the Riemannian distance to ∂M . By choosing specific $\phi \in \mathcal{D}$ as function of ρ_∂ , we obtain explicit Li-Yau type inequality from Theorem ?? with geometry quantities, by choosing test functions ℓ as in the proofs of Corollary ?? and Corollary ??.

Corollary 3.3. *Assume that (??) and (??) hold for some constants $K \in \mathbb{R}$ and $\sigma < 0$, and there exist constants $k, \theta, \sigma \geq 0$ and $r_0 > 0$ such that ρ_∂ is smooth on $\partial_{r_0} M := \{x \in M : \rho_\partial(x) \leq r_0\}$, $\mathbb{I} \leq \theta$, the sectional curvature of M on $\partial_{r_0} M$ is bounded above by k , and $|Z\rho_\partial|$ is bounded on $\partial_{r_0} M$. Let*

$$h_s := \cos \sqrt{k} s - \frac{\theta}{\sqrt{k}} \sin \sqrt{k} s, \quad s \geq 0,$$

$$\delta := -\frac{\sigma(1 - h_{r_0})^{d-1}}{\int_0^{r_0} (h_s - h_{r_0})^{d-1} ds},$$

$$\kappa := 1 + \delta \int_0^{r_0} (h_s - h_{r_0})^{1-d} \int_s^{r_0} (h_r - h_{r_0})^{d-1} dr,$$

$$\gamma := \delta(1 - h_{r_0})^{1-d} \int_0^{r_0} (h_s - h_{r_0})^{d-1} ds,$$

where for $k = 0$ the function h_s is defined by the limit as $k \downarrow 0$. Then (??) and (??) hold for $\|\phi\|_\infty = \kappa$, $\|\nabla \log \phi\|_\infty = \gamma$, and

$$K_\phi = -2(K - \delta + \sigma \|Z\rho_\partial\|_{\partial_{r_0} M}),$$

$$K_{\alpha,\phi} = -\frac{2\kappa^2(\delta - \sigma \|Z\rho_\partial\|_{\partial_{r_0} M} + K^-)}{\alpha - \kappa^2}, \quad \alpha > \kappa^2.$$

Proof. According to the proof of Theorem 3.2.9(2) in [?], we may choose $\phi = \varphi \circ \rho_\partial$, where

$$\varphi(r) := 1 + \delta \int_0^r (h_s - h_{r_0})^{1-d} \int_{s \wedge r_0}^{r_0} (h_a - h_{r_0})^{d-1} da ds, \quad r \geq 0.$$

Then $\frac{1}{\phi}\Delta\phi \geq -\delta$, so that

$$2\inf_M\{K + \phi^{-1}L\phi\} \geq -2(K - \delta + \sigma\|Z\rho_\partial\|_{\partial r_0 M});$$

$$\inf_M \frac{2(\phi L\phi + K\phi^2)}{\alpha - \phi^2} \geq -\frac{2\kappa^2(\delta - \sigma\|Z\rho_\partial\|_{\partial r_0 M} + K^-)}{\alpha - \kappa^2}.$$

□

4 Local Li-Yau Estimates

When M is non-compact and does not satisfy any conditions in Remark ??, to estimate $|\nabla u_t(x)|$ we may first restrict our calculus to a compact domain D containing x as an interior point, by using stochastic analysis as in the proof of Theorem ?? before the exit time of X_t from D . Under this restriction, we may estimate $|\nabla u_{t-s}(X_s)|$ by using bounded geometry quantities on D , so that the condition (??) is replaced by a suitable choice of the test function f satisfying (??) below.

Theorem 4.1. *Let $x \in M$, and let D be a compact domain in M such that $x \in D^o := D \setminus \partial D$ and when $D \cap \partial M \neq \emptyset$*

$$(4.1) \quad \sigma|_{D \cap \partial M} \geq 0.$$

Let $K_D \geq 0$ be a constant such that (??) holds on D for $K = -K_D$. Let $f \in C_b^2(D)$ such that

$$(4.2) \quad f|_D \leq 1, \quad f(x) = 1, \quad f|_{\partial D} = 0, \quad f|_{D^o} > 0, \quad Nf|_{D \cap \partial M} \geq 0,$$

where the condition $Nf|_{D \cap \partial M} \geq 0$ applies only when ∂M exists. Then the following estimates hold.

(1) *For any constant $\varepsilon > 0$, let*

$$\beta_{\varepsilon,f} := \sup_D \left\{ 2K_D - 2fLf + \left(6 + \frac{(1+\varepsilon)^2 n}{\varepsilon} \right) |\nabla f|^2 \right\}.$$

Then for any $t, \varepsilon > 0$,

$$(4.3) \quad \begin{aligned} \frac{|\nabla u_t|^2}{u_t^2}(x) &\leq \frac{n(1+\varepsilon)^2 \beta_{\varepsilon,f}}{2(1 - e^{-\beta_{\varepsilon,f} t})} \\ &+ \frac{2(1+\varepsilon)\beta_{\varepsilon,f} \int_0^t (e^{-2\beta_{\varepsilon,f}s} - e^{-\beta_{\varepsilon,f}(s+t)}) e^{2K_D s} ds}{(1 - e^{-\beta_{\varepsilon,f} t})^2} \frac{Lu_t}{u_t}(x). \end{aligned}$$

(2) *For any constant $\alpha > 1$, let*

$$\tilde{\beta}_{\alpha,f} := \sup_D \left\{ \left(6 + \frac{n\alpha^2}{\alpha - 1} \right) |\nabla f|^2 - 2fLf - \frac{2K_D}{\alpha - 1} f^2 \right\}.$$

Then for any $t > 0$,

$$(4.4) \quad \frac{|\nabla u_t|^2}{u_t^2}(x) \leq \alpha \frac{Lu_t}{u_t}(x) + \frac{n\alpha^2}{2} \left(\frac{K_D}{\alpha - 1} + \frac{\tilde{\beta}_{\alpha,f}}{1 - e^{-\tilde{\beta}_{\alpha,f} t}} \right).$$

Proof. (a) We follow the line of [?] by making a suitable time change $X_{\tau(t)}$ of the (reflecting) diffusion process X_t , where $\{\tau(t)\}_{t \geq 0}$ are stopping times satisfying

$$\tau(t) \leq \tau_D := \inf \{t \geq 0 : X_t \in \partial D\} < \infty \text{ a.s.}.$$

To this end, let

$$\begin{aligned} T(t) &:= \int_0^t f^{-2}(X_s) ds, \quad t \in [0, \tau_D], \\ \tau(t) &:= \inf \{s \geq 0 : T(s) \geq t\}, \quad t \geq 0. \end{aligned}$$

We have $T(\tau(t)) = t$ for all $t \geq 0$, $\tau(T(t)) = t$ for $t \in [0, \tau_D]$ and

$$(4.5) \quad dT(t) = f^{-2}(X_t) dt, \quad d\tau(t) = f^2(X_{\tau(t)}) dt.$$

The time-changed diffusion $X'_t := X_{\tau(t)}$ is generated by $L' := f^2 L$ which never hits the boundary ∂D , see [?].

Since $f \leq 1$, we have $T(t) \geq t$ and $\tau(t) \leq t$. For fixed $t > 0$, let

$$(4.6) \quad h_s := \frac{e^{-\beta_{\varepsilon,f}s} - e^{-\beta_{\varepsilon,f}t}}{1 - e^{-\beta_{\varepsilon,f}t}}, \quad s \in [0, t].$$

Then $h \in C_b^1([0, t])$ satisfies

$$(4.7) \quad h_0 = 1, \quad h_t = 0, \quad h''_s = -\beta_{\varepsilon,f} h'_s, \quad s \in [0, t].$$

By (??) with $\sigma \geq 0$ due to (??), (??) for $K = -K_D$, and Itô's formula since X is a solution to (??), we obtain

$$\begin{aligned} & d \left(h_s^2 e^{2K_D s} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) \right) \\ & \geq 2K_D (1 - f^2(X_{\tau(s)})) h_s^2 e^{2K_D s} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) ds \\ & \quad + 2h_s h'_s e^{2K_D s} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) ds \\ & \quad + \frac{2h_s^2 f^2}{nu_{t-\tau(s)}} (X_{\tau(s)}) e^{2K_D s} \left(Lu_{t-\tau(s)} - \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} \right)^2 (X_{\tau(s)}) ds. \end{aligned}$$

Noting that $f \leq 1$ and for any $\varepsilon \in (0, 1)$,

$$\begin{aligned} & 2h_s h'_s \frac{|\nabla u|^2}{u} + \frac{2h_s^2 f^2}{nu} \left(Lu - \frac{|\nabla u|^2}{u} \right)^2 \\ & = -2\varepsilon h_s h'_s \frac{|\nabla u|^2}{u} + 2(1 + \varepsilon) h_s h'_s Lu \\ & \quad + 2(1 + \varepsilon) h_s h'_s \left(\frac{|\nabla u|^2}{u} - Lu \right) + \frac{2h_s^2 f^2}{nu} \left(Lu - \frac{|\nabla u|^2}{u} \right)^2 \end{aligned}$$

$$\geq -2\varepsilon h_s h'_s \frac{|\nabla u|^2}{u} + 2(1+\varepsilon)h_s h'_s L u - \frac{n(1+\varepsilon)^2}{2}(h'_s)^2 u f^{-2},$$

we derive

$$\begin{aligned} & d \left(h_s^2 e^{2K_D s} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) \right) \\ & \stackrel{m}{\geq} \left(2(1+\varepsilon)h_s h'_s e^{2K_D s} L u_{t-\tau(s)} - 2\varepsilon h_s h'_s e^{2K_D s} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} \right) (X_{\tau(s)}) ds \\ & \quad - \frac{n(1+\varepsilon)^2}{2} e^{2K_D s} (h'_s)^2 (u_{t-\tau(s)} f^{-2}) (X_{\tau(s)}) ds. \end{aligned}$$

Since $dL u_{t-s}(X_s) \stackrel{m}{=} 0$ so that $\mathbb{E}^x[L u_{t-\tau(s)}(X_{\tau(s)})] = L u_t(x)$, combining this with $h_0 = 1, h_t = 0$ and $\tau(0) = 0$ implies

$$\begin{aligned} (4.8) \quad & \frac{|\nabla u_t|^2}{u_t}(x) \leq \frac{(1+\varepsilon)^2 n}{2} \mathbb{E}^x \int_0^t (h'_s)^2 e^{2K_D s} (f^{-2} u_{t-\tau(s)})(X_{\tau(s)}) ds \\ & - 2(1+\varepsilon)(L u_t(x)) \int_0^t h'_s h_s e^{2K_D s} ds + 2\varepsilon \mathbb{E}^x \int_0^t h'_s h_s e^{2K_D s} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) ds. \end{aligned}$$

To bound the first term in the right hand side, we apply Itô's formula to derive

$$\begin{aligned} & d \{ e^{(2K_D - \beta_{\varepsilon,f})s} f^{-2} u_{t-\tau(s)} \} (X_{\tau(s)}) \\ & \stackrel{m}{=} (-\beta_{\varepsilon,f} + 2K_D + f^4 L f^{-2}(X_{\tau(s)})) e^{(2K_D - \beta_{\varepsilon,f})s} u_{t-\tau(s)} (X_{\tau(s)}) f^{-2}(X_{\tau(s)}) ds \\ & \quad - 4e^{(2K_D - \beta_{\varepsilon,f})s} f^{-1}(X_{\tau(s)}) \langle \nabla f(X_{\tau(s)}), \nabla u_{t-\tau(s)}(X_{\tau(s)}) \rangle ds \\ & \leq e^{(2K_D - \beta_{\varepsilon,f})s} \left(-\beta_{\varepsilon,f} + 2K_D + f^4 L f^{-2} + \frac{n(1+\varepsilon)^2}{\varepsilon} |\nabla f|^2 \right) (f^{-2} u_{t-\tau(s)})(X_{\tau(s)}) ds \\ & \quad + \frac{4\varepsilon}{n(1+\varepsilon)^2} e^{(2K_D - \beta_{\varepsilon,f})s} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) ds \\ & \leq \frac{4\varepsilon}{n(1+\varepsilon)^2} e^{(2K_D - \beta_{\varepsilon,f})s} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) ds, \end{aligned}$$

where the last step follows from the fact that the definition of $\beta_{\varepsilon,f}$ implies

$$\beta_{\varepsilon,f} = \sup_D \left\{ 2K_D + f^4 L f^{-2} + \frac{n(1+\varepsilon)^2}{\varepsilon} |\nabla f|^2 \right\}.$$

Hence, by Gronwall's lemma and $f(X_0) = f(x) = 1$, we obtain

$$\begin{aligned} (4.9) \quad & \mathbb{E}^x \left[e^{2K_D s} (f^{-2} u_{t-\tau(s)})(X_{\tau(s)}) \right] \\ & \leq e^{\beta_{\varepsilon,f} s} u_t(x) + \frac{4\varepsilon e^{\beta_{\varepsilon,f} s}}{(1+\varepsilon)^2 n} \int_0^s e^{(2K_D - \beta_{\varepsilon,f})r} \mathbb{E}^x \left[\frac{|\nabla u_{t-\tau(r)}|^2}{u_{t-\tau(r)}} (X_{\tau(r)}) \right] dr. \end{aligned}$$

Since $h''_s = -\beta_{\varepsilon,f} h'_s$ due to (??), we obtain

$$(h_s h'_s e^{\beta_{\varepsilon,f} s})' = [(h'_s)^2 + h_s h''_s + \beta_{\varepsilon,f} h_s h'_s] e^{\beta_{\varepsilon,f} s} = (h'_s)^2 e^{\beta_{\varepsilon,f} s},$$

so the integration by parts formula yields

$$\begin{aligned} & \int_0^t (h'_s)^2 e^{\beta_{\varepsilon,f}s} \int_0^s e^{(2K_D - \beta_{\varepsilon,f})r} \mathbb{E}^x \left[\frac{|\nabla u_{t-\tau(r)}|^2}{u_{t-\tau(r)}} (X_{\tau(r)}) \right] dr ds \\ &= - \int_0^t h_s h'_s e^{2K_D s} \mathbb{E}^x \left[\frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) \right] ds. \end{aligned}$$

Combining this with (??) and (??), we arrive at

$$\frac{|\nabla u_t|^2}{u_t}(x) \leq \frac{n(1+\varepsilon)^2 u_t(x)}{2} \int_0^t (h'_s)^2 e^{\beta_{\varepsilon,f}s} ds - 2(1+\varepsilon)(Lu_t(x)) \int_0^t h'_s h_s e^{2K_D s} ds,$$

which implies the desired estimate (??) by the definition of h_s in (??).

(b) Recall that $\tilde{X}_s := X_{\tau(s)}$ is the diffusion process generated by $f^2 L$ on $D \setminus \partial D$. Let

$$K_f := \sup_D \{6|\nabla f|^2 - f L f\}.$$

By Itô's formula, we obtain

$$df^{-2}(\tilde{X}_s) \stackrel{m}{=} f^2 L f^{-2}(\tilde{X}_s) ds = f^{-2}(\tilde{X}_s) \{6|\nabla f|^2 - f L f\}(\tilde{X}_s) ds \leq K_f f^{-2}(\tilde{X}_s) ds.$$

This together with $f(\tilde{X}_0) = f(x) = 1$ yields

$$(4.10) \quad \mathbb{E}^x[f^{-2}(X_{\tau(s)})] \leq e^{K_f s}, \quad s \geq 0.$$

For any constant $\beta \geq 0$, let

$$(4.11) \quad \ell_s := \frac{e^{-\beta T(s \wedge \tau(t))} - e^{-\beta t}}{1 - e^{-\beta t}}, \quad s \in [0, t].$$

Then $\ell'_s \leq 0, \ell_s = 0$ for $s \geq \tau(t)$ where $\tau(t) \leq t \wedge \tau_D$. By (??), (??) and the integral transform $s = \tau(r)$, we obtain

$$\begin{aligned} (4.12) \quad & \mathbb{E}^x \left[\sup_{s \in [0, t]} \ell_s^2 \right] = \mathbb{E}^x \left[\sup_{s \in [0, t]} \left(\int_s^t \ell'_r dr \right)^2 \right] \\ & \leq t \mathbb{E}^x \int_0^t (\ell'_s)^2 ds = \frac{t\beta^2}{(1 - e^{-\beta t})^2} \mathbb{E}^x \int_0^{\tau(t)} e^{-2\beta T(s \wedge \tau(t))} f^{-4}(X_s) ds \\ &= \frac{t\beta^2}{(1 - e^{-\beta t})^2} \mathbb{E}^x \int_0^t e^{-2\beta r} f^{-2}(X_{\tau(r)}) dr < \infty. \end{aligned}$$

This implies that condition (??) holds, since $\frac{|\nabla u|^2}{u}$ is bounded on $[0, t] \times D$, $K^- = K_D$ on D , and $\sigma = 0$ on $D \cap \partial M$. So, by step (c) in the proof of Theorem ??, we obtain (??) for the present ℓ_s , i.e.

$$\begin{aligned} (4.13) \quad & \frac{|\nabla u_t|^2}{u_t}(x) \leq \alpha Lu_t(x) + \frac{n\alpha^2}{2} I_1 - (\alpha - 1) I_2, \\ & I_1 = \mathbb{E}^x \left[u_0(X_t) \int_0^{\tau(t)} e^{-\frac{2}{\alpha-1} K_D s} \left(\ell'_s - \frac{K_D}{\alpha-1} \ell_s \right)^2 ds \right], \\ & I_2 = 2 \mathbb{E}^x \left[\int_0^{\tau(t)} e^{-\frac{2}{\alpha-1} K_D s} |\ell_s \ell'_s| \frac{|\nabla u_{t-s}|^2}{u_{t-s}} (X_s) ds \right]. \end{aligned}$$

By (??) and the Markov property, we have

$$(4.14) \quad (Lu_{t-\tau(s)})(X_{\tau(s)}) = \mathbb{E}^x(Lu_0(X_t)|\mathcal{F}_{\tau(s)}), \quad u_{t-\tau(s)}(X_{\tau(s)}) = \mathbb{E}^x(u_0(X_t)|\mathcal{F}_{\tau(s)}).$$

Moreover, by $f \leq 1$, (??), (??), $\ell_0 = 1$, $\ell_{\tau(t)} = 0$ and the integral transform $s = \tau(r)$, we obtain

$$\begin{aligned} & \int_0^{\tau(t)} e^{-\frac{2K_D}{\alpha-1}s} \left(\ell'_s - \frac{K_D}{\alpha-1} \ell_s \right)^2 ds \\ &= \int_0^{\tau(t)} e^{-\frac{2K_D}{\alpha-1}s} (\ell'_s)^2 ds - 2 \frac{K_D}{\alpha-1} \int_0^{\tau(t)} e^{-\frac{2K_D}{\alpha-1}s} \ell'_s \ell_s ds + \left(\frac{K_D}{\alpha-1} \right)^2 \int_0^{\tau(t)} e^{-\frac{2K_D}{\alpha-1}s} \ell_s^2 ds \\ &= \int_0^{\tau(t)} e^{-\frac{2K_D}{\alpha-1}s} (\ell'_s)^2 ds + \frac{K_D}{\alpha-1} - \left(\frac{K_D}{\alpha-1} \right)^2 \int_0^{\tau(t)} e^{-\frac{2K_D}{\alpha-1}s} \ell_s^2 ds \\ &\leq \int_0^t \frac{\beta^2 e^{-2\beta r - \frac{2K_D}{\alpha-1}\tau(r)}}{(1 - e^{-\beta t})^2} f^{-2}(X_{\tau(r)}) dr + \frac{K_D}{\alpha-1}. \end{aligned}$$

Hence, (??) and (??) imply

$$(4.15) \quad I_1 \leq \frac{\beta^2}{(1 - e^{-\beta t})^2} \int_0^t \mathbb{E}^x \left[e^{-2\beta s - \frac{2K_D}{\alpha-1}\tau(s)} (f^{-2}u_{t-\tau(s)})(X_{\tau(s)}) \right] ds + \frac{K_D}{\alpha-1} u_t(x).$$

Similarly, by (??), (??) and the integral transform $s = \tau(r)$, we obtain

$$\begin{aligned} I_2 &= \frac{2\beta}{(1 - e^{-\beta t})^2} \int_0^t (e^{-2\beta s} - e^{-\beta(t+s)}) \mathbb{E}^x \left[e^{-\frac{2K_D}{\alpha-1}\tau(s)} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) \right] ds \\ (4.16) \quad &= \frac{2\beta^2}{(1 - e^{-\beta t})^2} \int_0^t e^{-\beta s} \left(\int_s^t e^{-\beta r} dr \right) \mathbb{E}^x \left[e^{-\frac{2K_D}{\alpha-1}\tau(s)} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) \right] ds \\ &= \frac{2\beta^2}{(1 - e^{-\beta t})^2} \int_0^t e^{-\beta r} dr \int_0^r e^{-\beta s} \mathbb{E}^x \left[e^{-\frac{2K_D}{\alpha-1}\tau(s)} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) \right] ds. \end{aligned}$$

Since $\tilde{X}_s := X_{\tau(s)}$ is generated by $f^2 L$, $u_{t-\tau(s)}(X_{\tau(s)})$ is a local martingale, and $\tau'(s) = f^2(X_{\tau(s)})$, by Itô's formula we obtain

$$\begin{aligned} & d \left(e^{-\beta s} e^{\frac{-2K_D\tau(s)}{\alpha-1}} (f^{-2}u_{t-\tau(s)})(X_{\tau(s)}) \right) \\ & \equiv \left(-\beta + f^4 L f^{-2}(X_{\tau(s)}) - \frac{2K_D}{\alpha-1} f^2(X_{\tau(s)}) \right) e^{-\beta s} e^{\frac{-2K_D\tau(s)}{\alpha-1}} (f^{-2}u_{t-\tau(s)})(X_{\tau(s)}) ds \\ & \quad - 4e^{-\beta s} e^{\frac{-2K_D\tau(s)}{\alpha-1}} f^{-1}(X_{\tau(s)}) \langle \nabla u_{t-\tau(s)}(X_{\tau(s)}), \nabla f(X_{\tau(s)}) \rangle ds \\ & \leq \left(-\beta + f^4 L f^{-2}(X_{\tau(s)}) + \frac{2}{\varepsilon} |\nabla f|^2(X_{\tau(s)}) - \frac{2K_D}{\alpha-1} f^2(X_{\tau(s)}) \right) e^{-\beta s} e^{\frac{-2K_D\tau(s)}{\alpha-1}} (f^{-2}u_{t-\tau(s)})(X_{\tau(s)}) ds \\ & \quad + 2\varepsilon e^{-\beta s} e^{\frac{-2K_D\tau(s)}{\alpha-1}} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} (X_{\tau(s)}) ds, \quad \varepsilon > 0. \end{aligned}$$

Choosing $\beta = \tilde{\beta}_{\alpha,f}$ and $\varepsilon = \frac{2(\alpha-1)}{n\alpha^2}$ such that

$$-\beta + f^4 L f^{-2}(X_{\tau(s)}) + \frac{2}{\varepsilon} |\nabla f|^2(X_{\tau(s)}) - \frac{2K_D}{\alpha-1} f^2(X_{\tau(s)}) \leq 0,$$

we derive

$$d\left(e^{-\beta s} e^{\frac{-2K_D\tau(s)}{\alpha-1}} (f^{-2}u_{t-\tau(s)})(X_{\tau(s)})\right) \stackrel{m}{\leq} \frac{4(\alpha-1)}{n\alpha^2} e^{-\beta s} e^{\frac{-2K_D\tau(s)}{\alpha-1}} \frac{|\nabla u_{t-\tau(s)}|^2}{u_{t-\tau(s)}} ds.$$

This together with $f(X_0) = f(x) = 1$ and $\tau(0) = 0$ yields

$$\begin{aligned} & \int_0^t \mathbb{E}^x \left[e^{-2\beta s - \frac{2K_D\tau(s)}{\alpha-1}} (f^{-2}u_{t-\tau(s)})(X_{\tau(s)}) \right] ds \\ & \leq u_t(x) \int_0^t e^{-\beta s} ds + \frac{4(\alpha-1)}{n\alpha^2} \int_0^t e^{-\beta s} ds \int_0^s e^{-\beta r} \mathbb{E}^x \left[e^{-\frac{2K_D}{\alpha-1}\tau(r)} \frac{|\nabla u_{t-\tau(r)}|^2}{u_{t-\tau(r)}} (X_{\tau(r)}) \right] dr. \end{aligned}$$

Combining this with (??), (??) and $\varepsilon = \frac{2(\alpha-1)}{n\alpha^2}$, we derive

$$\frac{n\alpha^2}{2} I_1 - (\alpha-1) I_2 \leq \frac{n\alpha^2}{2} \left(\frac{K_D}{\alpha-1} + \frac{\beta}{1-e^{-\beta t}} \right) u_t(x),$$

where $\beta = \tilde{\beta}_{\alpha,f}$. Then (??) follows from (??). \square

To derive explicit estimates from Theorem ??, we take $D = B(x, R)$, the geodesic ball in M centered at x with radius R , for any $R > 0$ and $x \in M$. Let

$$K_{x,R} := \inf \left\{ \text{Ric}_Z^{(n-m)}(v, v) : v \in \cup_{y \in B(x, R)} T_y M, |v| = 1 \right\}.$$

We have the following result.

Corollary 4.2. *Assume that ∂M is either convex or empty. Let $x \in M$ and $t > 0$. Then the following assertions hold.*

(1) *For any $\varepsilon \in (0, 1)$, (??) holds for $\beta_{\varepsilon,f}$ replaced by*

$$(4.17) \quad \beta_{\varepsilon,R} = 2K_{x,R} + \frac{\pi}{2R} \sqrt{K_{x,R}(n-1)} + \frac{\pi^2}{4R^2} \left[4 + (\varepsilon^{-1}(1+\varepsilon)^2 + 2)n \right].$$

(2) *For any $\alpha > 1$, (??) holds with $\tilde{\beta}_{\alpha,f}$ replaced by*

$$(4.18) \quad \tilde{\beta}_{\alpha,R} = \frac{\pi^2}{2R^2} \left(2 + n + \frac{n\alpha^2}{2(\alpha-1)} \right) + \frac{\pi}{2R} \sqrt{K_{x,R}(n-1)} + \frac{2K_{x,R}}{\alpha-1}.$$

Proof. Let $D = B(x, R)$, and let ρ_x be the Riemannian distance to point x . Choose

$$(4.19) \quad f = \cos \left(\frac{\pi \rho_x}{2R} \right).$$

Since ∂M is either convex or empty, we have $N\rho_x|_{\partial M} \leq 0$ so that f satisfies (??).

Next, by the curvature-dimension condition (??) on D for $K = -K_{x,R}$, and taking

$$\varphi(s) := \frac{\sinh(\sqrt{K_{x,R}/(n-1)}s)}{\sinh(\sqrt{K_{x,R}/(n-1)}\rho_x)}, \quad s \in [0, \rho_x],$$

in [?, (3)], we obtain the following Laplacian comparison theorem:

$$L\rho_x(y) \leq \sqrt{K_{x,R}(n-1)} \coth\left(\sqrt{K_{x,R}/(n-1)}\rho_x(y)\right), \quad x \neq y \in D \setminus \text{cut}(x),$$

where $\text{cut}(x)$ is the cut-locus of x , such that f is smooth on $D \setminus \text{cut}(x)$.

(a) When $\text{cut}(x) = \emptyset$, $f \in C_b^2(D)$ satisfying (??). Since ∂M is convex or empty, we have $\sigma = 0$. Combining these with $|\nabla \rho_x| = 1$, we conclude that $\beta_{\varepsilon,f}$ in Theorem ??(1) can be estimated:

$$\begin{aligned} \beta_{\varepsilon,f} &:= \sup_D \left\{ 2K_{x,R} - 2fLf + \left(6 + \frac{(1+\varepsilon)^2 n}{\varepsilon}\right) |\nabla f|^2 \right\} \\ &\leq \sup_{r \in [0, R]} \left\{ 2K_{x,R} + \frac{\pi}{2R} \sin\left(\frac{\pi r}{R}\right) \sqrt{K_{x,R}(n-1)} \coth\left(\sqrt{K_{x,R}/(n-1)} r\right) \right. \\ &\quad \left. + \frac{\pi^2}{2R^2} \cos^2\left(\frac{\pi r}{R}\right) + \left(6 + \frac{(1+\varepsilon)^2 n}{\varepsilon} \frac{\pi^2}{4R^2}\right) \sin^2\left(\frac{\pi r}{R}\right) \right\}. \end{aligned}$$

Noting that $\sin r \leq 1 \wedge r$, $\sin^2 r + \cos^2 r = 1$ and $\coth r \leq 1 + r^{-1}$ for $r > 0$, this implies

$$\begin{aligned} \beta_{\varepsilon,f} &\leq 2K_{x,R} + \frac{\pi}{2R} \left(\sqrt{K_{x,R}(n-1)} + \frac{\pi(n-1)}{R} \right) + \left(6 + \frac{n(1+\varepsilon)^2}{\varepsilon}\right) \frac{\pi^2}{4R^2} \\ &= 2K_{x,R} + \frac{\pi}{2R} \sqrt{K_{x,R}(n-1)} + \frac{\pi^2}{4R^2} \left[4 + (\varepsilon^{-1}(1+\varepsilon)^2 + 2)n \right]. \end{aligned}$$

So, by Theorem ??(1), (??) holds for $\beta_{\varepsilon,f}$ replaced by $\beta_{\varepsilon,R}$ in (??).

Similarly,

$$\begin{aligned} \tilde{\beta}_{\alpha,f} &:= \sup_D \left\{ \left(6 + \frac{n\alpha^2}{\alpha-1}\right) |\nabla f|^2 - 2fLf - \frac{2K_{x,R}}{\alpha-1} f^2 \right\} \\ &\leq \left(6 + \frac{n\alpha^2}{\alpha-1}\right) \frac{\pi^2}{4R^2} + \sup_{r \in [0, R]} \left\{ \frac{\pi}{2R} \sin\left(\frac{\pi r}{R}\right) \sqrt{K_{x,R}(n-1)} \coth\left(\sqrt{K_{x,R}/(n-1)} r\right) \right\} + \frac{2K_{x,R}}{\alpha-1} \\ &\leq \frac{\pi^2}{2R^2} \left(2 + n + \frac{n\alpha^2}{2(\alpha-1)}\right) + \frac{\pi}{2R} \sqrt{K_{x,R}(n-1)} + \frac{2K_{x,R}}{\alpha-1}. \end{aligned}$$

So, by Theorem ??(2), (??) holds for $\tilde{\beta}_{\alpha,f}$ replaced by $\tilde{\beta}_{\alpha,R}$ in (??).

(b) When $\text{cut}(x) \neq \emptyset$, noting that $N\rho_x|_{\partial M} \leq 0$ by the convexity of ∂M , the Itô formula for $\rho_x(X_t)$ due to [?] implies

$$\begin{aligned} d\rho_x(X_t) &\leq L\rho_x(X_t)dt + \sqrt{2}db_t \\ &\leq \sqrt{K_{x,R}(n-1)} \coth\left(\sqrt{K_{x,R}/(n-1)}\rho_x(X_t)\right) dt + \sqrt{2}db_t, \quad t \leq \tau_D, \end{aligned}$$

where b_t is the one-dimensional Brownian motion. With this inequality and the fact that $\cos r$ is smooth and decreasing in $r \in [0, \frac{\pi}{2}]$, the argument in the proof of Theorem ?? still works for the present choice of f , so that the proof is finished as in the above step (a). \square

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