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Gradient estimates for the heat equation on graphs

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Let $G(V,E)$ be an infinite (locally finite) graph which satisfies $CDE(m,-K)$ condition for some $m>0, K>0$. In this paper we mainly establish a generalized gradient estimate for positive solutions to the following heat equation

$$(\partial_t - \triangle_\mu)u = 0,$$

this gradient estimate includes Davies' estimate, Hamilton's estimate, Bakry-Qian's estimate and Li-Xu's estimate, these four estimates for positive solutions to the linear heat equation had been established on complete manifolds with Ricci curvature bounded from below by a negative number. When $t \searrow 0$, the dominant terms of Hamilton, Bakry-Qian and Li-Xu's estimates are consistent with the corresponding term on the case that $K = 0$. We can also derive the Harnack inequalities from the gradient estimates, and then obtain the heat kernel estimates.

1. Introduction

Li-Yau's famous gradient estimate for a positive solution u to the heat equation

$$(\partial_t - \triangle)u = 0, \tag{1.1}$$

established in [7], says that u satisfies

$$\frac{|\nabla u|^2}{u^2} - \alpha\frac{\partial_t u}{u} \le \frac{m\alpha^2 K}{2(\alpha-1)} + \frac{m\alpha^2}{2t} \tag{1.2}$$

on an $m-$dimensional complete Riemannian manifold (M,g) whose Ricci curvature is bounded from below by $-K$ for some constant $K \ge 0$, where

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$\alpha > 1$ is a given constant. In particular, u satisfies

$$\frac{|\nabla u|^2}{u^2} - \frac{\partial_t u}{u} \leq \frac{m}{2t} \tag{1.3}$$

if the Ricci curvature is nonnegative. The equality in (1.3) holds if u is the heat kernel on $\mathbf{R}^m$.

Li-Yau's gradient estimate can be used to derive the Harnack type inequalities, the upper and lower bound estimates for the heat kernel, the estimates of eigenvalues of the Laplace operator and the estimates of the Green's function on general complete Riemannian manifolds with Ricci curvature bounded from below. It has been playing great roles in the field of geometric analysis.

How to generalize the gradient estimate on manifolds to the graphic setting is an interesting question. The main difficulty is the lack of the chain rule on graphs. By using a crucial observation and a new version of the curvature-dimension condition, i.e., the $CDE(m, K)$ condition, the authors of [2] studied the Li-Yau's gradient estimate for positive solutions to the linear heat equation on the graphic setting, they also derived Harnack inequalities and heat kernel bounds from the gradient estimate. We state the gradient estimate in the graphic setting established in [2] as follows.

Theorem 1.1. *Let $G(V, E)$ be a (finite or infinite) graph satisfying $CDE(m, -K)$ condition for some constant $K \geq 0$, if $G(V, E)$ is infinite we also assume that it has bounded degree. Then for any positive function $u : V \times [0, +\infty) \to (0, +\infty)$ satisfying*

$$(\partial_t - \triangle_\mu) u = 0, \tag{1.4}$$

and any constant $\alpha > 1$,

$$\frac{\Gamma(\sqrt{u})}{u} - \alpha \frac{\partial_t \sqrt{u}}{\sqrt{u}} \leq \frac{m\alpha^2}{2t} + \frac{m\alpha^2 K}{2(\alpha - 1)} \tag{1.5}$$

holds on the whole graph, where $\triangle_\mu, \Gamma$ and $CDE(m, -K)$ condition are defined in Section 2. In particular, if $G(V, E)$ satisfies $CDE(m, 0)$ condition then

$$\frac{\Gamma(\sqrt{u})}{u} - \frac{\partial_t \sqrt{u}}{\sqrt{u}} \leq \frac{m}{2t} \tag{1.6}$$

holds on the whole graph.

In [4] Davies improved (1.2) to be

$$\frac{|\nabla u|^2}{u^2} - \alpha\frac{\partial_t u}{u} \leq \frac{m\alpha^2 K}{4(\alpha-1)} + \frac{m\alpha^2}{2t} \tag{1.7}$$

in the manifold setting. The dominant term of the right hand side of (1.7) is $\frac{m\alpha^2}{2t}$ when $t \searrow 0$. At the same time, the heat kernel on the $m-$dimensional hyperbolic space shows that the dominant term should be $\frac{m}{2t}$. If one lets $\alpha \searrow 1$, then the right hand side of (1.7) will blow up. An interesting question is: can one find a sharp gradient estimate form for positive solutions to the heat equation (1.2) on general manifolds with $\mathrm{Ric} \geq -K$? (see Problem 10.5 in book [3], page 393.) It seems difficult to solve this question completely. The author of [5] made some progress along this direction and got the following gradient estimate

$$\frac{|\nabla u|^2}{u^2} - e^{2Kt}\frac{\partial_t u}{u} \leq e^{4Kt}\frac{m}{2t}. \tag{1.8}$$

Later the linearized version

$$\frac{|\nabla u|^2}{u^2} - \left(1+\frac{2}{3}Kt\right)\frac{\partial_t u}{u} \leq \frac{m}{2t} + \frac{mK}{2}\left(1+\frac{1}{3}Kt\right) \tag{1.9}$$

was derived in [1]. But when $t \to \infty$, the righthand sides of (1.8) and (1.9) will blow up. Recently, a better estimate was given in [6], that is,

$$\frac{|\nabla u|^2}{u^2} - \left(1+\frac{\sinh Kt\cosh Kt - Kt}{\sinh^2 Kt}\right)\frac{\partial_t u}{u} \leq \frac{mK}{2}[\coth Kt + 1]. \tag{1.10}$$

It is easy to see that the righthand side of (1.10) stays bounded when $t \to \infty$.

In this paper, we can improve the estimate in (1.5) to be

$$\frac{\Gamma(\sqrt{u})}{u} - \alpha\frac{\partial_t\sqrt{u}}{\sqrt{u}} \leq \frac{m\alpha^2}{2t} + \frac{\alpha^2 mK}{4(\alpha-1)} \tag{1.11}$$

on a graph satisfying $CDE(m,-K)$ condition for some constant $K \geq 0$ (see Theorem 5.1). The dominant term of the right hand side of (1.11) is $\frac{m\alpha^2}{2t}$ when $t \searrow 0$. Note that the right hand side of (1.6) is $\frac{m}{2t}$. But if one lets $\alpha \searrow 1$, then the right hand side of (1.11) will blow up. A natural question is: can we establish gradient estimates similar to (1.8), (1.9) and (1.10) for positive solutions to the heat equation (1.4) on general graphs satisfying $CDE(m,-K)$ condition for some constant $K > 0$. The answer is affirmative and the following is the main result in this paper.

Theorem 1.2. *Let $G(V,E)$ be a (finite or infinite) graph satisfying $CDE(m,-K)$ condition for some constant $K>0$, if $G(V,E)$ is infinite we also assume that it has bounded degree. Then for any positive function $u : V \times [0,+\infty) \to (0,+\infty)$ satisfying (1.4) we have*

$$\frac{\Gamma(\sqrt{u})}{u} - e^{2Kt}\frac{\partial_t\sqrt{u}}{\sqrt{u}} \le e^{4Kt}\frac{m}{2t}, \tag{1.12}$$

$$\frac{\Gamma(\sqrt{u})}{u} - \left(1+\frac{2}{3}Kt\right)\frac{\partial_t\sqrt{u}}{\sqrt{u}} \le \frac{m}{2t} + \frac{mK}{2}\left(1+\frac{1}{3}Kt\right) \tag{1.13}$$

and

$$\frac{\Gamma(\sqrt{u})}{u} - \left(1+\frac{\sinh Kt\cosh Kt - Kt}{\sinh^2 Kt}\right)\frac{\partial_t\sqrt{u}}{\sqrt{u}} \le \frac{mK}{2}[\coth Kt + 1]. \tag{1.14}$$

This paper is organized as follows: In Section 2 we introduce some notations and lemmas, which will be used later. Then we establish a general form of Li-Yau's gradient estimate for positive solutions to the heat equation (1.4) on a (finite or infinite) graph satisfying $CDE(m,-K)$ condition for some constant $K>0$, the proof for the finite graph case is given in Section 3, and infinite graph case is given in Section 4. Then the Davies' gradient estimate (1.11), Hamilton's gradient estimate (1.12), Bakry-Qian's gradient estimate (1.13) and Li-Xu's gradient estimate (1.14) are all included in our general form. In fact, by choosing suitable $\alpha(t),\eta(t)$ and $\varphi(t)$ in Theorem 3.1 and Theorem 4.2, we can get gradient estimates (1.11), (1.12), (1.13) and (1.14) respectively, we explain these in Section 5. As applications we can derive the Harnack inequalities and the heat kernel estimates, we do these in Section 6 and Section 7 respectively.

2. Notations and lemmas

We firstly give some notations [2]. Let $G(V,E)$ be a graph whose edge $xy \in E$ from x to y has weight $w_{xy}>0$. We also assume that

$$w_{min} := \inf_{e\in E} w_e > 0 \tag{2.1}$$

and for all $x \in V$,

$$deg(x) := \sum_{y\sim x} w_{xy} < \infty, \tag{2.2}$$

i.e., the graph is locally finite. Given a measure $\mu : V \to \mathbf{R}$ on V, the μ-Laplacian on G is the operator $\triangle_\mu$ defined by

$$\triangle_\mu f(x) = \frac{1}{\mu(x)} \sum_{y\sim x} w_{xy}(f(y) - f(x)). \tag{2.3}$$

Moreover we define

$$D_w = \max_{x\sim y} \frac{deg(x)}{w_{xy}}, \tag{2.4}$$

$$D_\mu = \max_{x\in V} \frac{deg(x)}{\mu(x)}, \tag{2.5}$$

$$\begin{aligned} \Gamma(f,g)(x) &= \frac{1}{2}[\triangle_\mu(fg) - f\triangle_\mu g - g\triangle_\mu f](x) \\ &= \frac{1}{2}\frac{1}{\mu(x)} \sum_{y\sim x} w_{xy}(f(y) - f(x))(g(y) - g(x)) \end{aligned} \tag{2.6}$$

and

$$\Gamma_2(f,g) = \frac{1}{2}[\triangle_\mu \Gamma(f,g) - \Gamma(f, \triangle_\mu g) - \Gamma(\triangle_\mu f, g)]. \tag{2.7}$$

For convenience, we write $\Gamma(f) = \Gamma(f,f), \Gamma_2(f) = \Gamma_2(f,f)$.

When studying gradient estimates on manifolds we always need the following identity

$$\triangle_\mu \ln u = \frac{\triangle_\mu u}{u} - |\nabla \ln u|^2,$$

which comes from the chain rule formula. However the chain rule formula is always false in the graphic setting. In [2] the authors observed that in the graphic setting the identity

$$2\sqrt{u}\triangle_\mu \sqrt{u} = \triangle_\mu u - 2\Gamma(\sqrt{u}) \tag{2.8}$$

is right. In order to establish Li-Yau's gradient estimate, they also introduced the following $CDE(m,K)$ condition.

Definition 2.1. We say that a graph $G(V,E)$ satisfies $CDE(m,K)$ condition, if for all $x \in V$, any positive function $f : V \to \mathbf{R}$ such that $(\triangle_\mu f)(x) <$

0 we have

$$\tilde{\Gamma}_2(f)(x) \geq \frac{1}{m}(\triangle_\mu f)^2(x) + K\Gamma(f)(x), \tag{2.9}$$

where

$$\begin{aligned} \tilde{\Gamma}_2(f) &= \Gamma_2(f) - \Gamma\left(f, \frac{\Gamma(f)}{f}\right) \\ &= \frac{1}{2}\triangle_\mu\Gamma(f) - \frac{1}{2}\Gamma\left(f, \frac{\triangle_\mu f^2}{f}\right). \end{aligned} \tag{2.10}$$

The following maximum principle, which is established in [2], is useful.

Lemma 2.2. *Let $G(V,E)$ be a (finite or infinite) graph, and let $g, F : V \times [0,T] \to \mathbf{R}$ be two functions. Suppose that $g(x,t) \geq 0$, and $f(x,t)$ has a local maximum at $(x_0,t_0) \in V \times [0,T]$. Further assume that $t_0 \neq 0$. Then*

$$\mathcal{L}(gf)(x_0,t_0) \leq (\mathcal{L}g)(x_0,t_0)f(x_0,t_0), \tag{2.11}$$

where $\mathcal{L} = \triangle_\mu - \partial_t$.

We also need the following inequality [2].

Lemma 2.3. *Assume that $f : V \to \mathbf{R}$ satisfies $f > 0$ and $(\triangle_\mu f)(x) < 0$ at some vertex x. Then we have*

$$\frac{1}{\mu(x)}\sum_{y\sim x} w_{xy} f(y) < D_\mu f(x) \tag{2.12}$$

and

$$\frac{1}{\mu(x)}\sum_{y\sim x} w_{xy} f^2(y) < D_\mu D_w f^2(x). \tag{2.13}$$

3. Gradient estimate on finite graphs

We assume that $\alpha(t) > 1, \eta(t) \geq 0$ and $\varphi(t) \geq 0$ are smooth functions defined on $[0,+\infty)$ and satisfy the following conditions:

$$(\alpha(t)-1)^2\eta'(t) - (\alpha(t)-1)(\alpha'(t)-2K)\eta(t) - \frac{m}{4}(\alpha'(t)-2K\alpha(t))^2 = 0, \tag{3.1}$$

$$\varphi(0) = 0 \tag{3.2}$$

and

$$m\alpha^2\varphi\left[\frac{\varphi'}{\varphi}+\frac{\alpha'}{\alpha}-\frac{2\eta}{m\alpha^2}\right]$$

is nonnegative and nondecreasing about t.

Before proving (1.11) and Theorem 1.2, we firstly establish a generalized gradient estimate for positive solutions to (1.4), then (1.11) and Theorem 1.2 will be derived by choosing suitable $\alpha(t), \eta(t)$ and $\varphi(t)$. In this section we consider the case that the graph is finite.

Theorem 3.1. *Let $G(V,E)$ be a finite graph satisfying $CDE(m,-K)$ condition for some constant $K>0$. Then for any positive function $u: V\times[0,+\infty)\to(0,+\infty)$ satisfying (1.4),*

$$\frac{\Gamma(\sqrt{u})}{u}-\alpha(t)\frac{\partial_t\sqrt{u}}{\sqrt{u}}\le-\frac{\eta(t)}{2}+\frac{m\alpha^2(t)}{2}\left[\frac{\varphi'(t)}{\varphi(t)}+\frac{\alpha'(t)}{\alpha(t)}\right] \tag{3.3}$$

holds on the whole graph.

Proof. Let

$$F=\varphi(t)\left(\frac{2\Gamma(\sqrt{u})-\alpha(t)\triangle_\mu u}{u}-\eta(t)\right). \tag{3.4}$$

By (2.8) we have

$$\begin{aligned} F&=\varphi(t)\left(\frac{2(1-\alpha)\Gamma(\sqrt{u})}{u}-\frac{2\alpha(t)\triangle_\mu\sqrt{u}}{\sqrt{u}}-\eta(t)\right)\\ &\le-\frac{2\varphi(t)\alpha(t)\triangle_\mu\sqrt{u}}{\sqrt{u}}. \end{aligned} \tag{3.5}$$

For any $T>0$ fixed, we assume that at $(x_0,t_0)\in V\times[0,T]$, F achieves its maximum on $V\times[0,T]$. We may assume that $F(x_0,t_0)>0$, otherwise there is nothing to prove. Hence $t_0>0$ and $\triangle_\mu\sqrt{u}(x_0,t_0)<0$. In what follows all computations are understood at the point (x_0,t_0). We apply Lemma 2.2

with the choice of $g = u$. This gives

$$
\begin{aligned}
(3.6)\qquad 0 &= \mathcal{L}(u)F \geq \mathcal{L}(uF) = \mathcal{L}[\varphi(t)(2\Gamma(\sqrt{u}) - \alpha(t)\triangle_\mu u - \eta(t)u)] \\
&= (\triangle_\mu - \partial_t)[\varphi(t)(2\Gamma(\sqrt{u}) - \alpha(t)\triangle_\mu u - \eta(t)u)] \\
&= 2\varphi(t)\triangle_\mu \Gamma(\sqrt{u}) - \varphi(t)\alpha(t)\triangle_\mu\triangle_\mu u - \varphi(t)\eta(t)\triangle_\mu u \\
&\quad - \varphi'(t)(2\Gamma(\sqrt{u}) - \alpha(t)\triangle_\mu u - \eta(t)u) - 4\varphi(t)\Gamma\left(\sqrt{u}, \frac{\partial_t u}{2\sqrt{u}}\right) \\
&\quad + \varphi(t)(\alpha(t)\partial_t(\triangle_\mu u) + \alpha'(t)\triangle_\mu u + \eta'(t)u + \eta(t)\partial_t u).
\end{aligned}
$$

By using (1.4), (2.10) and (2.9), we have

$$
\begin{aligned}
(3.7)\qquad 0 &\geq 4\varphi(t)\tilde{\Gamma}_2(\sqrt{u}) - \frac{\varphi'(t)}{\varphi(t)}uF + \varphi(t)\alpha'(t)\triangle_\mu u + \varphi(t)\eta'(t)u \\
&\geq \frac{4\varphi(t)}{m}(\triangle_\mu\sqrt{u})^2 - 4\varphi(t)K\Gamma(\sqrt{u}) - \frac{\varphi'(t)}{\varphi(t)}uF \\
&\quad + \varphi(t)\alpha'(t)\triangle_\mu u + \varphi(t)\eta'(t)u.
\end{aligned}
$$

By (3.4) and (2.8) we know that

$$
(3.8)\qquad \triangle_\mu u = \frac{2\Gamma(\sqrt{u})}{\alpha(t)} - \frac{\eta(t)u}{\alpha(t)} - \frac{uF}{\alpha(t)\varphi(t)},
$$

$$
(3.9)\qquad \triangle_\mu \sqrt{u} = \frac{1-\alpha(t)}{\alpha(t)}\frac{\Gamma(\sqrt{u})}{\sqrt{u}} - \frac{\eta(t)\sqrt{u}}{2\alpha(t)} - \frac{\sqrt{u}F}{2\alpha(t)\varphi(t)}.
$$

Plugging (3.8) and (3.9) into (3.7) leads to

$$
\begin{aligned}
(3.10)\qquad 0 &\geq \frac{uF^2}{m\alpha^2(t)\varphi(t)} + \frac{4(\alpha(t)-1)}{m\alpha^2(t)}\Gamma(\sqrt{u})F \\
&\quad + \left(\frac{2\eta(t)}{m\alpha^2(t)} - \frac{\varphi'(t)}{\varphi(t)} - \frac{\alpha'(t)}{\alpha(t)}\right)uF \\
&\quad + \frac{4(1-\alpha(t))^2\varphi(t)}{m\alpha^2(t)}\frac{(\Gamma(\sqrt{u}))^2}{u} \\
&\quad + \left(\frac{\varphi(t)\eta^2(t)}{m\alpha^2(t)} - \frac{\varphi(t)\alpha'(t)\eta(t)}{\alpha(t)} + \varphi(t)\eta'(t)\right)u \\
&\quad + \left[\frac{4\varphi(t)(\alpha(t)-1)\eta(t)}{m\alpha^2(t)} - 4K\varphi(t) + \frac{2\varphi(t)\alpha'(t)}{\alpha(t)}\right]\Gamma(\sqrt{u}).
\end{aligned}
$$

A direct calculation shows that (3.1) is equivalent to

$$\begin{aligned}(3.11)\qquad &\left[\frac{4\varphi(t)(\alpha(t)-1)\eta(t)}{m\alpha^2(t)} - 4K\varphi(t) + \frac{2\varphi(t)\alpha'(t)}{\alpha(t)}\right]^2\\ &= \frac{16(1-\alpha(t))^2\varphi(t)}{m\alpha^2(t)}\left[\frac{\varphi(t)\eta^2(t)}{m\alpha^2(t)} - \frac{\varphi(t)\alpha'(t)\eta(t)}{\alpha(t)} + \varphi(t)\eta'(t)\right].\end{aligned}$$

Hence

$$\begin{aligned}(3.12)\qquad &\frac{4(1-\alpha(t))^2\varphi(t)}{m\alpha^2(t)}\frac{(\Gamma(\sqrt{u}))^2}{u}\\ &+\left(\frac{\varphi(t)\eta^2(t)}{m\alpha^2(t)} - \frac{\varphi(t)\alpha'(t)\eta(t)}{\alpha(t)} + \varphi(t)\eta'(t)\right)u\\ &+\left[\frac{4\varphi(t)(\alpha(t)-1)\eta(t)}{m\alpha^2(t)} - 4K\varphi(t) + \frac{2\varphi(t)\alpha'(t)}{\alpha(t)}\right]\Gamma(\sqrt{u}) \geq 0.\end{aligned}$$

We then get that

$$\begin{aligned}(3.13)\qquad 0 &\geq \frac{uF^2}{m\alpha^2(t)\varphi(t)} + \frac{4(\alpha(t)-1)}{m\alpha^2(t)}\Gamma(\sqrt{u})F\\ &\quad+\left(\frac{2\eta(t)}{m\alpha^2(t)} - \frac{\varphi'(t)}{\varphi(t)} - \frac{\alpha'(t)}{\alpha(t)}\right)uF\\ &\geq \frac{uF^2}{m\alpha^2(t)\varphi(t)} + \left(\frac{2\eta(t)}{m\alpha^2(t)} - \frac{\varphi'(t)}{\varphi(t)} - \frac{\alpha'(t)}{\alpha(t)}\right)uF.\end{aligned}$$

Hence

$$\begin{aligned}(3.14)\qquad F(x_0,t_0) &\leq m\alpha^2(t_0)\varphi(t_0)\left[\frac{\varphi'(t_0)}{\varphi(t_0)} + \frac{\alpha'(t_0)}{\alpha(t_0)} - \frac{2\eta(t_0)}{m\alpha^2(t_0)}\right]\\ &\leq m\alpha^2(T)\varphi(T)\left[\frac{\varphi'(T)}{\varphi(T)} + \frac{\alpha'(T)}{\alpha(T)} - \frac{2\eta(T)}{m\alpha^2(T)}\right],\end{aligned}$$

here the second inequality comes from the fact that

$$m\alpha^2\varphi\left[\frac{\varphi'}{\varphi} + \frac{\alpha'}{\alpha} - \frac{2\eta}{m\alpha^2}\right]$$

is nonnegative and nondecreasing about t. Hence for all $x \in V$,

$$F(x,T) \leq F(x_0,t_0) \leq m\alpha^2(T)\varphi(T)\left[\frac{\varphi'(T)}{\varphi(T)} + \frac{\alpha'(T)}{\alpha(T)} - \frac{2\eta(T)}{m\alpha^2(T)}\right],$$

or

$$\frac{\Gamma(\sqrt{u})}{u}(x,T)-\alpha(T)\frac{\partial_t\sqrt{u}}{\sqrt{u}}(x,T)\le-\frac{\eta(T)}{2}+\frac{m\alpha^2(T)}{2}\left[\frac{\varphi'(T)}{\varphi(T)}+\frac{\alpha'(T)}{\alpha(T)}\right].$$

Then (3.3) holds since $T>0$ is arbitrary. □

4. Gradient estimate on infinite graphs

We assume that $\alpha(t)>1,\eta(t)\ge 0$ and $\varphi(t)\ge 0$ are smooth functions and satisfy conditions in Theorem 3.1. In this section we establish the following generalized gradient estimate on an infinite graph by using the cutoff function.

Theorem 4.1. *Let $G(V,E)$ be an infinite graph satisfying $CDE(m,-K)$ condition for some constant $K>0$. Then for any positive function $u:V\times[0,+\infty)\to(0,+\infty)$ satisfying (1.4),*

$$\frac{\Gamma(\sqrt{u})}{u}-\alpha(t)\frac{\partial_t\sqrt{u}}{\sqrt{u}}\le-\frac{\eta(t)}{2}+\frac{m\alpha^2(t)}{2}\left[\frac{\varphi'(t)}{\varphi(t)}+\frac{\alpha'(t)}{\alpha(t)}\right]+\frac{2}{R}\frac{\theta(t)}{\varphi(t)} \tag{4.1}$$

holds at (x,t) satisfying $d(x,O)<R$, where $d(x,O)$ denotes the distance from x to a fixed point O and

$$\theta(t)=\max_{\tau\in[0,t]}\{mD_\mu D_w\alpha^2(\tau)\varphi(\tau)+D_\mu\alpha(\tau)\varphi(\tau)\}. \tag{4.2}$$

Proof. The cutoff function $\phi:V\to\mathbf{R}$ is defined by

$$\phi(x)=\begin{cases}0, & d(x,O)>2R\\ \frac{2R-d(x,O)}{R} & 2R\ge d(x,O)\ge R\\ 1 & R\ge d(x,O).\end{cases}$$

Let

$$G(x,t)=\phi(x)F(x,t)=\phi(x)\varphi(t)\left(\frac{2\Gamma(\sqrt{u})-\alpha(t)\triangle_\mu u}{u}-\eta(t)\right). \tag{4.3}$$

By (3.5) we have

$$G(x,t)\le-\frac{2\phi(x)\varphi(t)\alpha(t)\triangle_\mu\sqrt{u}}{\sqrt{u}}. \tag{4.4}$$

For any $T>0$ fixed, we assume that at $(x_0,t_0)\in V\times[0,T]$, G achieves its maximum on $V\times[0,T]$. We can also assume that $G(x_0,t_0)>0$. Due to (4.4) we have that $\phi(x_0)\varphi(t_0) > 0$ and $\triangle_\mu \sqrt{u}(x_0, t_0) < 0$. Let us first assume that $\phi(x_0) = \frac{1}{R}$. Since u is positive, by Lemma 2.3 we have that at (x_0, t_0),

$$-\frac{\triangle_\mu \sqrt{u}}{\sqrt{u}} = \frac{1}{\mu(x_0)} \sum_{y \sim x_0} w_{x_0 y} \left(1 - \frac{\sqrt{u}(y)}{\sqrt{u}(x_0)}\right) \leq D_\mu.$$

Together with (4.4) we have that at (x_0, t_0),

$$\begin{aligned} G(x_0, t_0) &\leq -\phi(x_0) \frac{2\varphi(t_0)\alpha(t_0)\triangle_\mu \sqrt{u}}{\sqrt{u}} \\ &\leq 2\phi(x_0)\varphi(t_0)\alpha(t_0) D_\mu = \frac{2\varphi(t_0)\alpha(t_0) D_\mu}{R}. \end{aligned}$$

We have that for all $x \in V$ so that $d(x, O) < R$,

$$\begin{aligned} F(x, T) = \phi(x) F(x, T) &= G(x, T) \leq G(x_0, t_0) \\ &\leq \frac{2\varphi(t_0)\alpha(t_0) D_\mu}{R} \leq \frac{2\theta(T)}{R}, \end{aligned}$$

and dividing by $\varphi(T)$ yields a stronger result than desired. Therefore we may assume that $\phi(x_0) \geq \frac{2}{R}$ and ϕ does not vanish in the neighborhood of x_0. In what follows all computations are understood at the point (x_0, t_0). We apply Lemma 2.2 and get

$$\begin{aligned} \mathcal{L}\left(\frac{u}{\phi}\right) G \geq \mathcal{L}\left(\frac{u}{\phi} G\right) &= \mathcal{L}[\varphi(t)(2\Gamma(\sqrt{u}) - \alpha(t)\triangle_\mu u - \eta(t) u)] \\ &\geq \frac{u F^2}{m\alpha^2(t)\varphi(t)} + \left(\frac{2\eta(t)}{m\alpha^2(t)} - \frac{\varphi'(t)}{\varphi(t)} - \frac{\alpha'(t)}{\alpha(t)}\right) u F, \end{aligned} \tag{4.5}$$

where the second inequality comes from the proof of Theorem 3.1. By (1.4) we have

$$\mathcal{L}\left(\frac{u}{\phi}\right)(x_0, t_0) = \frac{1}{\mu(x_0)} \sum_{y \sim x_0} w_{x_0 y} \left(\frac{1}{\phi(y)} - \frac{1}{\phi(x_0)}\right) u(y, t_0).$$

Let's write $\phi(x_0) = \frac{s}{R}$, then for any $y \sim x_0$, $\phi(y) = \frac{s \pm 1}{R}$, or $\phi(y) = \frac{s}{R}$. In any case

$$\left|\frac{1}{\phi(y)} - \frac{1}{\phi(x_0)}\right| \leq \frac{R}{s(s-1)}.$$

Hence

$$\begin{aligned}\mathcal{L}\left(\frac{u}{\phi}\right)(x_0,t_0) &\le \frac{R}{s(s-1)}\frac{1}{\mu(x_0)}\sum_{y\sim x_0} w_{x_0y}u(y,t_0)\\ &= \frac{Ru(x_0,t_0)}{s(s-1)}\frac{1}{\mu(x_0)}\sum_{y\sim x_0} w_{x_0y}\frac{u(y,t_0)}{u(x_0,t_0)}\\ &\le \frac{Ru(x_0,t_0)}{s(s-1)}D_\mu D_w,\end{aligned} \tag{4.6}$$

where in the last inequality we have used Lemma 2.3. Plugging (4.6) into (4.5) and dividing by $\frac{u}{\phi^2}$ leads to

$$\begin{aligned}&\frac{G^2}{m\alpha^2(t)\varphi(t)} + \left(\frac{2\eta(t)}{m\alpha^2(t)} - \frac{\varphi'(t)}{\varphi(t)} - \frac{\alpha'(t)}{\alpha(t)}\right)G\phi\\ &\le \frac{R}{s(s-1)}D_\mu D_w\phi^2 G = \frac{1}{R}\frac{s}{s-1}D_\mu D_w G \le \frac{2}{R}D_\mu D_w G.\end{aligned}$$

Since $0 \le \phi \le 1$ and

$$m\alpha^2\varphi\left[\frac{\varphi'}{\varphi} + \frac{\alpha'}{\alpha} - \frac{2\eta}{m\alpha^2}\right]$$

is nonnegative and nondecreasing about t, we have that

$$\begin{aligned}G(x_0,t_0) &\le m\alpha^2(t_0)\varphi(t_0)\left[\frac{\varphi'(t_0)}{\varphi(t_0)} + \frac{\alpha'(t_0)}{\alpha(t_0)} - \frac{2\eta(t_0)}{m\alpha^2(t_0)} + \frac{2}{R}D_\mu D_w\right]\\ &\le m\alpha^2(T)\varphi(T)\left[\frac{\varphi'(T)}{\varphi(T)} + \frac{\alpha'(T)}{\alpha(T)} - \frac{2\eta(T)}{m\alpha^2(T)}\right]\\ &\quad + \frac{2m}{R}D_\mu D_w\alpha^2(t_0)\varphi(t_0)\\ &\le m\alpha^2(T)\varphi(T)\left[\frac{\varphi'(T)}{\varphi(T)} + \frac{\alpha'(T)}{\alpha(T)} - \frac{2\eta(T)}{m\alpha^2(T)}\right] + \frac{2\theta(T)}{R}.\end{aligned}$$

We then get that for all $x \in V$ satisfying $d(x,O) < R$,

$$\begin{aligned}F(x,T) &= \phi(x)F(x,T) = G(x,T) \le G(x_0,t_0)\\ &\le m\alpha^2(T)\varphi(T)\left[\frac{\varphi'(T)}{\varphi(T)} + \frac{\alpha'(T)}{\alpha(T)} - \frac{2\eta(T)}{m\alpha^2(T)}\right] + \frac{2\theta(T)}{R},\end{aligned}$$

or

$$\begin{aligned}&\frac{\Gamma(\sqrt{u})}{u}(x,T)-\alpha(T)\frac{\partial_t\sqrt{u}}{\sqrt{u}}(x,T)\\ &\le -\frac{\eta(T)}{2}+\frac{m\alpha^2(T)}{2}\left[\frac{\varphi'(T)}{\varphi(T)}+\frac{\alpha'(T)}{\alpha(T)}\right]+\frac{2}{R}\frac{\theta(T)}{\varphi(T)}.\end{aligned}$$

Then (4.1) holds since $T>0$ is arbitrary. □

Theorem 4.2. *Let $G(V,E)$ be an infinite graph satisfying $CDE(m,-K)$ condition for some constant $K>0$, we also assume that $G(V,E)$ has bounded degree. Then for any positive function $u : V\times[0,+\infty)\to(0,+\infty)$ satisfying (1.4),*

$$\frac{\Gamma(\sqrt{u})}{u}-\alpha(t)\frac{\partial_t\sqrt{u}}{\sqrt{u}}\le -\frac{\eta(t)}{2}+\frac{m\alpha^2(t)}{2}\left[\frac{\varphi'(t)}{\varphi(t)}+\frac{\alpha'(t)}{\alpha(t)}\right] \tag{4.7}$$

holds on the whole graph.

Proof. By letting $R\to\infty$ in (4.1) we will get (4.7). □

5. Several special gradient estimates

In this section we will derive Davies' gradient estimate, Hamilton's gradient estimate, Bakry-Qian's gradient estimate and Li-Xu's gradient estimate. We firstly state the Davies' gradient estimate.

Theorem 5.1. *Let $G(V,E)$ be a (finite or infinite) graph satisfying $CDE(m,-K)$ condition for some constant $K\ge 0$, if $G(V,E)$ is infinite we also assume that it has bounded degree. Then for any positive function $u : V\times[0,+\infty)\to(0,+\infty)$ satisfying (1.4) and any constant $\alpha>1$,*

$$\frac{\Gamma(\sqrt{u})}{u}-\alpha\frac{\partial_t\sqrt{u}}{\sqrt{u}}\le\frac{m\alpha^2}{2t}+\frac{\alpha^2 mK}{4(\alpha-1)} \tag{5.1}$$

holds on the whole graph.

Proof. The proof relies on a refined discussion. We choose

$$\varphi(t)=t,\quad \alpha(t)=\alpha>1,\quad \eta(t)=-\frac{mK\alpha^2}{2(\alpha-1)}\le 0$$

in the proof of Theorem 4.1. That is,

$$G(x,t) = \phi(x)t\left(\frac{2\Gamma(\sqrt{u}) - \alpha\triangle_\mu u}{u} + \frac{mK\alpha^2}{2(\alpha-1)}\right) \tag{5.2}$$
$$\leq -\frac{2\phi(x)\varphi(t)\alpha\triangle_\mu\sqrt{u}}{\sqrt{u}} + \frac{mK\alpha^2\phi(x)t}{2(\alpha-1)}.$$

For any $T > 0$ fixed, we assume that at $(x_0, t_0) \in V \times [0, T]$, G achieves its maximum on $V \times [0, T]$. If

$$G(x_0, t_0) \leq \frac{mK\alpha^2 T}{2(\alpha-1)},$$

then for all $x \in V$ satisfying $d(x, O) < R$,

$$F(x, T) = G(x, T) \leq G(x_0, t_0) \leq \frac{mK\alpha^2 T}{2(\alpha-1)},$$

where

$$F(x,t) = t\left(\frac{2\Gamma(\sqrt{u}) - \alpha\triangle_\mu u}{u} + \frac{mK\alpha^2}{2(\alpha-1)}\right),$$

or

$$\frac{2\Gamma(\sqrt{u}) - \alpha\triangle_\mu u}{u} + \frac{mK\alpha^2}{2(\alpha-1)} \leq \frac{mK\alpha^2}{2(\alpha-1)}. \tag{5.3}$$

Now we assume that

$$G(x_0, t_0) > \frac{mK\alpha^2 T}{2(\alpha-1)}.$$

Due to (5.2) we have that $\phi(x_0)\varphi(t_0) > 0$ and $\triangle_\mu\sqrt{u}(x_0, t_0) < 0$. If $\phi(x_0) = \frac{1}{R}$, a similar discussion as in the proof of Theorem 4.1 shows that for all $x \in V$ satisfying $d(x, O) < R$,

$$\frac{2\Gamma(\sqrt{u}) - \alpha\triangle_\mu u}{u} + \frac{mK\alpha^2}{2(\alpha-1)} \leq \frac{2\alpha D_\mu}{R}. \tag{5.4}$$

Therefore we may assume that $\phi(x_0) \geq \frac{2}{R}$ and ϕ does not vanish in the neighborhood of x_0. In what follows all computations are understood at the point (x_0, t_0). From (4.5) we have

$$\mathcal{L}\left(\frac{uG}{\phi}\right) = \mathcal{L}(uF) \tag{5.5}$$
$$\geq \frac{uF^2}{m\alpha^2 t} - \left(\frac{K}{\alpha-1} - \frac{1}{t}\right) uF + \frac{4(1-\alpha)^2 t}{m\alpha^2}\frac{(\Gamma(\sqrt{u}))^2}{u}$$
$$+ \frac{mK^2\alpha^2}{4(\alpha-1)^2} tu + \left[\frac{4(\alpha-1)F}{m\alpha^2} - 6Kt\right]\Gamma(\sqrt{u}).$$

If

$$F \geq \frac{m\alpha^2 Kt}{\alpha-1},$$

then

$$\mathcal{L}\left(\frac{uG}{\phi}\right) \geq \frac{uF^2}{m\alpha^2 t} - \left(\frac{K}{\alpha-1} + \frac{1}{t}\right) uF + \frac{4(1-\alpha)^2 t}{m\alpha^2}\frac{(\Gamma(\sqrt{u}))^2}{u}$$
$$+ \frac{mK^2\alpha^2}{4(\alpha-1)^2} tu - 2Kt\Gamma(\sqrt{u}).$$

It is easy to verify that

$$\frac{4(1-\alpha)^2 t}{m\alpha^2}\frac{(\Gamma(\sqrt{u}))^2}{u} + \frac{mK^2\alpha^2}{4(\alpha-1)^2} tu - 2Kt\Gamma(\sqrt{u}) \geq 0.$$

Due to Lemma 2.2 we have

$$\mathcal{L}\left(\frac{u}{\phi}\right) G \geq \mathcal{L}\left(\frac{uG}{\phi}\right) \geq \frac{uF^2}{m\alpha^2 t} - \left(\frac{K}{\alpha-1} + \frac{1}{t}\right) uF.$$

Let's write $\phi(x_0) = \frac{s}{R}$, by using (4.6) we have

$$\frac{2uD_\mu D_w G}{R\phi^2} \geq \frac{uF^2}{m\alpha^2 t} - \left(\frac{K}{\alpha-1} + \frac{1}{t}\right) uF.$$

Hence

$$G(x_0, t_0) \leq \frac{m\alpha^2 K t_0}{\alpha-1} + m\alpha^2 + \frac{2m\alpha^2 D_\mu D_w t_0}{R}. \tag{5.6}$$

If

$$F \leq \frac{m\alpha^2 Kt}{\alpha-1},$$

then

$$G = \phi F \leq F \leq \frac{m\alpha^2 Kt}{\alpha - 1},$$

and (5.6) also holds. Hence for all $x \in V$ satisfying $d(x, O) < R$, we have

$$F(x, T) \leq \frac{m\alpha^2 KT}{\alpha - 1} + m\alpha^2 + \frac{2m\alpha^2 D_\mu D_w T}{R},$$

or

$$\frac{2\Gamma(\sqrt{u}) - \alpha\triangle_\mu u}{u} + \frac{mK\alpha^2}{2(\alpha - 1)} \leq \frac{m\alpha^2 K}{\alpha - 1} + \frac{m\alpha^2}{T} + \frac{2m\alpha^2 D_\mu D_w}{R}. \tag{5.7}$$

It is easy to see that both (5.3) and (5.4) are included in (5.7). Since $T > 0$ is arbitrary, we can arrive at (5.1) by letting $R \to \infty$ in (5.7). □

By choosing suitable $\alpha(t), \eta(t)$ and $\varphi(t)$ in Theorem 3.1 and Theorem 4.2, we can get Hamilton's gradient estimate, Bakry-Qian's gradient estimate and Li-Xu's gradient estimate, i.e., Theorem 1.2. Now let's prove Theorem 1.2.

Proof. For (1.12), we choose

$$\alpha(t) = e^{2Kt}, \ \eta(t) = 0, \ \varphi(t) = te^{-2Kt}.$$

If $K > 0$, then α, η and φ satisfy (3.1) and (3.2). A calculation shows that

$$\frac{m\alpha^2\varphi}{2}\left[\frac{\varphi'}{\varphi} + \frac{\alpha'}{\alpha} - \frac{4\eta}{m\alpha^2}\right] = \frac{me^{2Kt}}{2},$$

which is nonnegative and nondecreasing about t. Then (1.12) follows from (3.3) and (4.7).

For (1.13), we choose

$$\alpha(t) = 1 + \frac{2}{3}Kt, \quad \eta(t) = \frac{m}{t} + mK\left(1 + \frac{1}{3}Kt\right),$$
$$\varphi(t) = t^2 \exp\left(-\frac{1}{3}\int_0^t \frac{4K + 2K^2 s}{\alpha^2(s)}\,\mathrm{d}s\right).$$

Then α, η and φ satisfy (3.1) and (3.2). A calculation shows that

$$\frac{m\alpha^2\varphi}{2}\left[\frac{\varphi'}{\varphi} + \frac{\alpha'}{\alpha} - \frac{4\eta}{m\alpha^2}\right] = 0.$$

Then (1.13) follows from (3.3) and (4.7).

For (1.14), we choose

$$\alpha(t) = 1 + \frac{\sinh Kt \cosh Kt - Kt}{\sinh^2 Kt},$$
$$\eta(t) = mK(\coth Kt + 1)$$

and

$$\varphi(t) = \frac{\alpha(t_0)\varphi(t_0)}{\alpha(t)} \exp\left(\frac{2}{m}\int_{t_0}^{t} \frac{\eta(s)}{\alpha^2(s)}\, \mathrm{d}s\right),$$

here $t_0 > 0$ is a given constant small enough and $\varphi(t_0)$ is a given positive constant. Direct calculation shows that α, η and φ satisfy (3.1) and

$$\frac{m\alpha^2\varphi}{2}\left[\frac{\varphi'}{\varphi} + \frac{\alpha'}{\alpha} - \frac{2\eta}{m\alpha^2}\right] = 0.$$

Now we verify (3.2). There exists $\varsigma \in (t_0, t)$ so that

$$\begin{aligned}
\varphi(t) &= \frac{\alpha(t_0)\varphi(t_0)}{\alpha(t)} \exp\left(\frac{2}{m\alpha^2(\varsigma)}\int_{t_0}^{t} \eta(s)\, \mathrm{d}s\right)\\
&= \frac{\alpha(t_0)\varphi(t_0)}{\alpha(t)} \exp\left[\frac{2}{m\alpha^2(\varsigma)}\left(\frac{m}{2}\ln\frac{\sinh Kt}{\sinh Kt_0} + \frac{mK}{2}(t-t_0)\right)\right]\\
&= \frac{\alpha(t_0)\varphi(t_0)}{\alpha(t)}\left(\frac{\sinh Kt}{\sinh Kt_0}\right)^{\frac{1}{\alpha^2(\varsigma)}} e^{\frac{K(t-t_0)}{\alpha^2(\varsigma)}}.
\end{aligned}$$

Since $\alpha(t) \to 1$ as $t \searrow 0$. We can assume that $0.5 \le \frac{1}{\alpha^2(\varsigma)} \le 1$. Hence

$$\lim_{t\searrow 0}\varphi(t) = \lim_{t\searrow 0}\frac{\alpha(t_0)\varphi(t_0)}{\alpha(t)}\left(\frac{\sinh Kt}{\sinh Kt_0}\right)^{\frac{1}{\alpha^2(\varsigma)}} e^{\frac{K(t-t_0)}{\alpha^2(\varsigma)}} = 0.$$

Then (1.14) follows from (3.3) and (4.7). □

6. Harnack inequality

As in the manifold setting, we can also derive the Harnack inequality from gradient estimates (3.3) and (4.7). We firstly give a lemma which will be used later.

Lemma 6.1. *For any constants $c>0, 0<T_1<T_2$, any functions $\alpha\geq 1$ and ψ defined on $[T_1,T_2]$, we have*

$$\min_{s\in[T_1,T_2]}\left[\psi(s)-\frac{1}{c}\int_s^{T_2}\frac{\psi^2(t)}{\alpha(t)}\ \mathrm{d}t\right]\leq\frac{c}{(T_1-T_2)^2}\int_{T_1}^{T_2}\alpha(t)\ \mathrm{d}t. \tag{6.1}$$

Proof.

$$\begin{aligned}
&\min_{s\in[T_1,T_2]}\left[\psi(s)-\frac{1}{c}\int_s^{T_2}\frac{\psi^2(t)}{\alpha(t)}\ \mathrm{d}t\right]\\
&\leq\frac{\int_{T_1}^{T_2}\frac{2}{c}(s-T_1)[\psi(s)-\frac{1}{c}\int_s^{T_2}\frac{\psi^2(t)}{\alpha(t)}\ \mathrm{d}t]\ \mathrm{d}s}{\int_{T_1}^{T_2}\frac{2}{c}(s-T_1)\ \mathrm{d}s}\\
&=\frac{c}{(T_1-T_2)^2}\left[\int_{T_1}^{T_2}\frac{2}{c}(s-T_1)\psi(s)\ \mathrm{d}s-\frac{1}{c}\int_{T_1}^{T_2}\frac{\psi^2(t)}{\alpha(t)}\int_{T_1}^{t}\frac{2}{c}(s-T_1)\ \mathrm{d}s\ \mathrm{d}t\right]\\
&=\frac{1}{(T_1-T_2)^2}\int_{T_1}^{T_2}\left[2(t-T_1)\psi(t)-\frac{(t-T_1)^2}{c}\frac{\psi^2(t)}{\alpha(t)}\right]\ \mathrm{d}t\\
&\leq\frac{c}{(T_1-T_2)^2}\int_{T_1}^{T_2}\alpha(t)\ \mathrm{d}t,
\end{aligned}$$

here the last inequality comes from the fact that $-ax^2+bx\leq\frac{b^2}{4a}$ holds for $a>0$. □

We assume that $\alpha(t)>1, \eta(t)\geq 0$ and $\varphi(t)\geq 0$ are smooth functions and satisfy conditions in Theorem 3.1 on a finite graph, or conditions in Theorem 4.2 on an infinite graph. Now we state the main result in this section.

Theorem 6.2. *Let $G(V,E)$ be a (finite or infinite) graph satisfying $CDE(m,-K)$ condition for some constant $K>0$, if $G(V,E)$ is infinite we also assume that it has bounded degree and bounded measure $\mu\leq\mu_{max}$. Then for any positive function $u: V\times[0,+\infty)\to(0,+\infty)$ satisfying (1.4) we have*

$$\frac{\sqrt{u}(x,T_1)}{\sqrt{u}(y,T_2)}\leq\exp\left[\int_{T_1}^{T_2}\frac{\tilde{\eta}(t)}{\alpha(t)}\ \mathrm{d}t+\frac{\mu_{max}d^2(x,y)}{2w_{min}(T_1-T_2)^2}\int_{T_1}^{T_2}\alpha(t)\ \mathrm{d}t\right], \tag{6.2}$$

where

$$\tilde{\eta}(t)=-\frac{\eta(t)}{2}+\frac{m\alpha^2(t)}{2}\left[\frac{\varphi'(t)}{\varphi(t)}+\frac{\alpha'(t)}{\alpha(t)}\right]. \tag{6.3}$$

Proof. We firstly assume that $x \sim y$. Then for any $s \in [T_1, T_2]$,

$$\begin{aligned}
&\ln \sqrt{u}(x,T_1) - \ln \sqrt{u}(y,T_2) \\
&= \ln \frac{\sqrt{u}(x,T_1)}{\sqrt{u}(x,s)} + \ln \frac{\sqrt{u}(x,s)}{\sqrt{u}(y,s)} + \ln \frac{\sqrt{u}(y,s)}{\sqrt{u}(y,T_2)} \\
&= -\int_{T_1}^{s} \partial_t \ln \sqrt{u}(x,t)\ \mathrm{d}t + \ln \frac{\sqrt{u}(x,s)}{\sqrt{u}(y,s)} - \int_{s}^{T_2} \partial_t \ln \sqrt{u}(y,t)\ \mathrm{d}t.
\end{aligned}$$

By (3.3) and (4.7) we have

$$-\partial_t \ln \sqrt{u}(x,t) = -\frac{\partial_t \sqrt{u}}{\sqrt{u}}(x,t) \leq \frac{\tilde{\eta}(t)}{\alpha(t)} - \frac{1}{\alpha(t)} \frac{\Gamma(\sqrt{u})}{u}(x,t).$$

Note that for any $a, b > 0$, $\ln \frac{b}{a} \leq \frac{b-a}{a}$, we then get

$$\begin{aligned}
&\ln \sqrt{u}(x,T_1) - \ln \sqrt{u}(y,T_2) \\
&\leq \int_{T_1}^{T_2} \frac{\tilde{\eta}(t)}{\alpha(t)}\ \mathrm{d}t + \ln \frac{\sqrt{u}(x,s)}{\sqrt{u}(y,s)} \\
&\quad - \left(\int_{T_1}^{s} \frac{1}{\alpha(t)} \frac{\Gamma(\sqrt{u})}{u}(x,t)\ \mathrm{d}t + \int_{s}^{T_2} \frac{1}{\alpha(t)} \frac{\Gamma(\sqrt{u})}{u}(y,t)\ \mathrm{d}t \right) \\
&\leq \int_{T_1}^{T_2} \frac{\tilde{\eta}(t)}{\alpha(t)}\ \mathrm{d}t + \frac{\sqrt{u}(x,s) - \sqrt{u}(y,s)}{\sqrt{u}(y,s)} - \int_{s}^{T_2} \frac{1}{\alpha(t)} \frac{\Gamma(\sqrt{u})}{u}(y,t)\ \mathrm{d}t.
\end{aligned}$$

Since $y \sim x$, the definition of Γ shows that

$$\Gamma(\sqrt{u})(y,t) \geq \frac{w_{min}}{2\mu_{max}} (\sqrt{u}(x,t) - \sqrt{u}(y,t))^2.$$

Hence

$$\begin{aligned}
\ln \sqrt{u}(x,T_1) - \ln \sqrt{u}(y,T_2) \leq& \int_{T_1}^{T_2} \frac{\tilde{\eta}(t)}{\alpha(t)}\ \mathrm{d}t + \frac{\sqrt{u}(x,s) - \sqrt{u}(y,s)}{\sqrt{u}(y,s)} \\
&- \int_{s}^{T_2} \frac{w_{min}}{2\mu_{max}\alpha(t)} \frac{(\sqrt{u}(x,t) - \sqrt{u}(y,t))^2}{u(y,t)}\ \mathrm{d}t.
\end{aligned}$$

We choose s so that the right hand side is minimal. Lemma 6.1 tells us that

$$\begin{aligned}
&\ln \sqrt{u}(x,T_1) - \ln \sqrt{u}(y,T_2) \\
&\leq \int_{T_1}^{T_2} \frac{\tilde{\eta}(t)}{\alpha(t)}\ \mathrm{d}t + \frac{\mu_{max}}{2w_{min}(T_1 - T_2)^2} \int_{T_1}^{T_2} \alpha(t)\ \mathrm{d}t.
\end{aligned} \tag{6.4}$$

When x and y are not adjacent, we simply choose $x = x_0, x_1, \dots, x_k = y$ to be a path between x and y so that $k = d(x, y)$, and let $T_1 = t_0 < t_1 < \dots < t_k = T_2$ to be a subdivision of the time interval $[T_1, T_2]$ into k equal parts. Then

$$
\begin{aligned}
(6.5)\qquad & \ln\sqrt{u}(x, T_1) - \ln\sqrt{u}(y, T_2) \\
&= \sum_{i=0}^{k-1} [\ln\sqrt{u}(x_i, t_i) - \ln\sqrt{u}(x_{i+1}, t_{i+1})] \\
&\le \sum_{i=0}^{k-1} \left[\int_{t_i}^{t_{i+1}} \frac{\tilde{\eta}(t)}{\alpha(t)}\, \mathrm{d}t + \frac{\mu_{max}}{2w_{min}(t_{i+1} - t_i)^2} \int_{t_i}^{t_{i+1}} \alpha(t)\, \mathrm{d}t \right] \\
&= \int_{T_1}^{T_2} \frac{\tilde{\eta}(t)}{\alpha(t)}\, \mathrm{d}t + \frac{\mu_{max} k^2}{2w_{min}(T_1 - T_2)^2} \int_{T_1}^{T_2} \alpha(t)\, \mathrm{d}t.
\end{aligned}
$$

By (6.4) and (6.5) we have that

$$
\begin{aligned}
(6.6)\qquad & \ln\sqrt{u}(x, T_1) - \ln\sqrt{u}(y, T_2) \\
&\le \int_{T_1}^{T_2} \frac{\tilde{\eta}(t)}{\alpha(t)}\, \mathrm{d}t + \frac{\mu_{max} d^2(x, y)}{2w_{min}(T_1 - T_2)^2} \int_{T_1}^{T_2} \alpha(t)\, \mathrm{d}t,
\end{aligned}
$$

which implies (6.2). □

We easily get the following four Harnack inequalities.

Theorem 6.3. *Let $G(V, E)$ be a (finite or infinite) graph satisfying $CDE(m, -K)$ condition for some constant $K > 0$, if $G(V, E)$ is infinite we also assume that it has bounded degree and bounded measure $\mu \le \mu_{max}$. Assume that $u : V \times [0, +\infty) \to (0, +\infty)$ satisfying (1.4). Then for any constant $\alpha > 1$,*

$$
(6.7)\qquad \frac{\sqrt{u}(x, T_1)}{\sqrt{u}(y, T_2)} \le \left(\frac{T_2}{T_1}\right)^{\frac{m\alpha}{2}} \exp\left[\frac{m\alpha K(T_2 - T_1)}{4(\alpha - 1)} + \frac{\alpha \mu_{max} d^2(x, y)}{2w_{min}(T_2 - T_1)}\right],
$$

$$
(6.8)\qquad \frac{\sqrt{u}(x, T_1)}{\sqrt{u}(y, T_2)} \le \exp\left[\int_{T_1}^{T_2} \frac{me^{2Kt}}{2t}\, \mathrm{d}t + \frac{\mu_{max} d^2(x, y)(e^{2KT_2} - e^{2KT_1})}{4Kw_{min}(T_1 - T_2)^2}\right],
$$

$$
\begin{aligned}
(6.9)\qquad \frac{\sqrt{u}(x, T_1)}{\sqrt{u}(y, T_2)} &\le \left(\frac{T_2}{T_1}\right)^{\frac{m}{2}} \left[\frac{1 + \frac{2}{3}KT_2}{1 + \frac{2}{3}KT_1}\right]^{-\frac{1}{8}} \\
&\quad \times \exp\left[\frac{mK}{4}(T_2 - T_1) + \frac{\mu_{max} d^2(x, y)}{w_{min}} \frac{1 + \frac{K}{3}(T_1 + T_2)}{T_2 - T_1}\right]
\end{aligned}
$$

and

$$\frac{\sqrt{u}(x,T_1)}{\sqrt{u}(y,T_2)} \le \left(\frac{e^{2KT_2}-2KT_2-1}{e^{2KT_1}-2KT_1-1}\right)^{\frac{m}{4}}$$

$$\times \exp\left[\frac{\mu_{max}d^2(x,y)}{2w_{min}(T_2-T_1)}\left(1+\frac{T_2\coth KT_2 - T_1\coth KT_1}{T_2-T_1}\right)\right]. \tag{6.10}$$

Proof. By using (5.1), we have

$$-\partial_t \ln\sqrt{u}(x,t) \le \frac{m\alpha}{2t} + \frac{mK\alpha}{4(\alpha-1)} - \frac{1}{\alpha}\frac{\Gamma(\sqrt{u})}{u}(x,t).$$

A discussion similar to the proof of (6.2) leads to

$$\ln\sqrt{u}(x,T_1) - \ln\sqrt{u}(y,T_2)$$
$$\le \frac{m\alpha}{2}\ln\frac{T_2}{T_1} + \frac{mK\alpha}{4(\alpha-1)}(T_2-T_1) + \frac{\mu_{max}d^2(x,y)}{2w_{min}(T_1-T_2)^2}\int_{T_1}^{T_2}\alpha(t)\ \mathrm{d}t,$$

which implies (6.7).

In order to prove (6.8), we let

$$\alpha(t) = e^{2Kt}, \quad \eta(t) = 0, \quad \varphi(t) = te^{-2Kt}.$$

Then $\tilde{\eta}(t) = \frac{me^{4Kt}}{2t}$, and (6.8) comes from (6.2).

In order to prove (6.9), we let

$$\alpha(t) = 1+\frac{2}{3}Kt, \quad \eta(t) = \frac{m}{t} + mK\left(1+\frac{1}{3}Kt\right),$$
$$\varphi(t) = t^2\exp\left(-\frac{1}{3}\int_0^t \frac{4K+2K^2s}{\alpha^2(s)}\ \mathrm{d}s\right).$$

A calculation shows that

$$\tilde{\eta}(t) = \frac{m}{2t} + \frac{1}{2}mK + \frac{1}{6}mK^2t,$$

and (6.9) comes from (6.2).

In order to prove (6.10), we let

$$\alpha(t) = 1 + \frac{\sinh Kt \cosh Kt - Kt}{\sinh^2 Kt},$$
$$\eta(t) = mK(\coth Kt + 1)$$

and

$$\varphi(t) = \frac{\alpha(t_0)\varphi(t_0)}{\alpha(t)} \exp\left(\frac{2}{m}\int_{t_0}^{t} \frac{\eta(s)}{\alpha^2(s)}\,\mathrm{d}s\right),$$

here $t_0 > 0$ is a given constant small enough and $\varphi(t_0)$ is a given positive constant. A calculation shows that $\tilde{\eta}(t) = \frac{1}{2}\eta(t)$, and (6.10) comes from (6.2). □

7. Heat kernel estimates

In [7], based on Li-Yau's gradient estimate, the authors derived heat kernel estimates in the manifold setting. We assume that $\alpha(t) > 1, \eta(t) \geq 0$ and $\varphi(t) \geq 0$ are smooth functions and satisfy conditions in Theorem 3.1 on a finite graph, or conditions in Theorem 4.2 on an infinite graph. Let's state the following heat kernel estimate in the graphic setting.

Theorem 7.1. *Let $G(V,E)$ be a (finite or infinite) graph satisfying $CDE(m,-K)$ condition for some constant $K > 0$, if $G(V,E)$ is infinite we also assume that it has bounded degree and bounded measure $\mu \leq \mu_{max}$. Then there exist absolute constants $C_1, C_2 > 0$, so that the heat kernel $H(x,y,t)$ associated to the heat equation (1.4) both satisfies the lower bound estimate*

$$H(x,y,t) \geq C_1 \exp\left[-2\int_1^t \frac{\tilde{\eta}(t)}{\alpha(t)}\,\mathrm{d}t - \frac{\mu_{max} d^2(x,y)}{w_{min}(t-1)^2}\int_1^t \alpha(t)\,\mathrm{d}t\right] \tag{7.1}$$

for $t > 1$, and the upper bound estimate

$$H(x,y,t) \leq \frac{C_2 \mu(y)}{Vol(B(x,\sqrt{t}))} \times \exp\left[2\int_t^{2t} \frac{\tilde{\eta}(t)}{\alpha(t)}\,\mathrm{d}t + \frac{\mu_{max} d^2(x,y)}{w_{min} t}\int_t^{2t} \alpha(t)\,\mathrm{d}t\right] \tag{7.2}$$

for $t > 0$, where

$$Vol(B(x,\sqrt{t})) = \sum_{z \in B(x,\sqrt{t})} \mu(z).$$

Proof. By the Harnack inequality (6.2) we get that

$$\frac{\sqrt{H(x,x,1)}}{\sqrt{H(x,y,t)}} \leq \exp\left[\int_1^t \frac{\tilde{\eta}(t)}{\alpha(t)}\ \mathrm{d}t + \frac{\mu_{max} d^2(x,y)}{2w_{min}(t-1)^2} \int_1^t \alpha(t)\ \mathrm{d}t\right].$$

Then (7.1) holds due to the fact that $H(x,x,1)$ is bounded from below by an absolute constant $\sqrt{C_1}$ in a bounded degree graph.

For the upper bound estimate in (7.2), we get from (6.2) that

$$\frac{\sqrt{H(x,y,t)}}{\sqrt{H(z,y,2t)}} \leq \exp\left[\int_t^{2t} \frac{\tilde{\eta}(t)}{\alpha(t)}\ \mathrm{d}t + \frac{\mu_{max} d^2(x,z)}{2w_{min} t^2} \int_t^{2t} \alpha(t)\ \mathrm{d}t\right].$$

Then

$$\begin{aligned}
(7.3)\quad H(x,y,t) &\leq \frac{1}{Vol(B(x,\sqrt{t}))} \sum_{z\in B(x,\sqrt{t})} \mu(z) \Bigg[H(z,y,2t) \\
&\quad \times \exp\left(2\int_t^{2t} \frac{\tilde{\eta}(t)}{\alpha(t)}\ \mathrm{d}t + \frac{\mu_{max} d^2(x,z)}{w_{min} t^2} \int_t^{2t} \alpha(t)\ \mathrm{d}t\right)\Bigg] \\
&\leq \frac{1}{Vol(B(x,\sqrt{t}))} \exp\Bigg(2\int_t^{2t} \frac{\tilde{\eta}(t)}{\alpha(t)}\ \mathrm{d}t \\
&\quad + \frac{\mu_{max}}{w_{min} t} \int_t^{2t} \alpha(t)\ \mathrm{d}t\Bigg) \sum_{z\in B(x,\sqrt{t})} \mu(z) H(z,y,2t) \\
&\leq \frac{C_2 \mu(y)}{Vol(B(x,\sqrt{t}))} \exp\left(2\int_t^{2t} \frac{\tilde{\eta}(t)}{\alpha(t)}\mathrm{d}t + \frac{\mu_{max}}{w_{min} t} \int_t^{2t} \alpha(t)\mathrm{d}t\right),
\end{aligned}$$

here the last inequality comes from the fact that [2]

$$\sum_{z\in B(x,\sqrt{t})} \mu(z) H(z,y,2t) \leq C_2 \mu(y),$$

where C_2 is an absolute constant. □

Based on Theorem 6.3, we can derive the following heat kernel estimates.

Theorem 7.2. *Let $G(V,E)$ be a (finite or infinite) graph satisfying $CDE(m,-K)$ condition for some constant $K > 0$, if $G(V,E)$ is infinite we also assume that it has bounded degree and bounded measure $\mu \leq \mu_{max}$. Then* *there exist absolute constants $C_1, C_2 > 0$, so that the heat kernel $H(x,y,t)$ associated to the heat equation (1.4) both satisfies the lower bound estimates*

$$H(x,y,t) \geq C_1 t^{-m\alpha} \exp\left[-\frac{m\alpha K(t-1)}{2(\alpha-1)} - \frac{\alpha\mu_{max} d^2(x,y)}{w_{min}(t-1)}\right], \tag{7.4}$$

$$H(x,y,t) \geq C_1 \exp\left[-\int_1^t \frac{me^{2Kt}}{t}\,\mathrm{d}t - \frac{\mu_{max} d^2(x,y)(e^{2Kt}-e^{2K})}{2Kw_{min}(t-1)^2}\right], \tag{7.5}$$

$$H(x,y,t) \geq C_1 t^{-m} \left[\frac{1+\frac{2}{3}Kt}{1+\frac{2}{3}K}\right]^{\frac{1}{4}} \times \exp\left[-\frac{mK}{2}(t-1) - \frac{2\mu_{max} d^2(x,y)}{w_{min}} \frac{1+\frac{K}{3}(t+1)}{t-1}\right], \tag{7.6}$$

$$H(x,y,t) \geq C_1 \left(\frac{e^{2Kt}-2Kt-1}{e^{2K}-2K-1}\right)^{-\frac{m}{2}} \times \exp\left[-\frac{\mu_{max} d^2(x,y)}{w_{min}(t-1)} \left(1+\frac{t\coth Kt - \coth K}{t-1}\right)\right] \tag{7.7}$$

for $t > 1$, and the upper bound estimates

$$H(x,y,t) \leq \frac{2^{m\alpha} C_2 \mu(y)}{Vol(B(x,\sqrt{t}))} \exp\left[\frac{m\alpha Kt}{2(\alpha-1)} + \frac{\alpha\mu_{max} d^2(x,y)}{w_{min} t}\right], \tag{7.8}$$

$$H(x,y,t) \leq \frac{C_2 \mu(y)}{Vol(B(x,\sqrt{t}))} \times \exp\left[\int_t^{2t} \frac{me^{2Kt}}{t}\,\mathrm{d}t + \frac{\mu_{max} d^2(x,y)(e^{4Kt}-e^{2Kt})}{2Kw_{min} t^2}\right], \tag{7.9}$$

$$H(x,y,t) \leq \frac{C_2 \mu(y)}{Vol(B(x,\sqrt{t}))} 2^m \left[\frac{1+\frac{4}{3}Kt}{1+\frac{2}{3}Kt}\right]^{-\frac{1}{4}} \times \exp\left[\frac{mK}{2} t + \frac{2\mu_{max} d^2(x,y)}{w_{min}} \frac{1+Kt}{t}\right], \tag{7.10}$$

$$H(x,y,t) \leq \frac{C_2 \mu(y)}{Vol(B(x,\sqrt{t}))} \left(\frac{e^{4Kt}-4Kt-1}{e^{2Kt}-2Kt-1}\right)^{\frac{m}{2}} \times \exp\left[\frac{\mu_{max} d^2(x,y)}{w_{min} t} \left(1+\frac{2t\coth 2Kt - t\coth Kt}{t}\right)\right] \tag{7.11}$$

for $t > 0$.

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