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LI-YAU INEQUALITY ON GRAPHS

Frank Bauer, Paul Horn, Yong Lin, Gabor Lippner,
Dan Mangoubi & Shing-Tung Yau

Abstract

We prove the Li-Yau gradient estimate for the heat kernel on graphs. The only assumption is a variant of the curvature-dimension inequality, which is purely local, and can be considered as a new notion of curvature for graphs. We compute this curvature for lattices and trees and conclude that it behaves more naturally than the already existing notions of curvature. Moreover, we show that if a graph has non-negative curvature then it has polynomial volume growth.

We also derive Harnack inequalities and heat kernel bounds from the gradient estimate, and show how it can be used to derive a Buser-type inequality relating the spectral gap and the Cheeger constant of a graph.

1. Introduction and main ideas

In their celebrated work [**19**] Li and Yau proved an upper bound on the gradient of positive solutions of the heat equation. In its simplest form, for an n-dimensional compact manifold with non-negative Ricci curvature the Li-Yau gradient estimate states that a positive solution u of the heat equation $(\Delta - \partial_t)u = 0$ satisfies

$$|\nabla \log u|^2 - \partial_t(\log u) = \frac{|\nabla u|^2}{u^2} - \frac{\partial_t u}{u} \leq \frac{n}{2t}. \tag{1.1}$$

The inequality (1.1) has been generalized to many important settings in geometric analysis. The most notable such generalization was made by Hamilton on the Ricci flow; see [**14**, **15**].

Finding a discrete version of (1.1) has proven challenging for a long time. Indeed, there is no graph for which inequality (1.1) is true for all times t (cf. §4.1). The main difficulty for finding a discrete version is that the chain rule *fails* on graphs. In this paper, we succeed in finding an analogue of inequality (1.1) on graphs. The main breakthrough and novelty of this paper, as we see, are twofold. First, we show a way to bypass the chain rule in the discrete setting. The way we do it (as explained in §1.1), we believe, may be adapted to many other

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circumstances. Second, we introduce a new natural notion of curvature of graphs, modifying the curvature notion of [**20**]. For example, we are able to prove a discrete version of the Li-Yau inequality where the curvature is bounded from below (by any real number). Also, we show that non-negatively curved graphs have polynomial growth. As far as we are aware of, this result, well known on Riemannian manifolds, is not known with any previous notion of curvature on graphs.

In the next two sections we explain the preceding two ideas in more detail.

1.1. Bypassing the chain rule—discretizing the logarithm. In proving the gradient estimate (1.1) on manifolds, either by the maximum principle [**19**] or by semigroup methods [**4**], it is crucial to have the chain rule in hand. Namely, both proofs use a simple but a key identity that follows from the chain rule formula:

$$\Delta \log u = \frac{\Delta u}{u} - |\nabla \log u|^2. \tag{1.2}$$

However, this is false in the discrete setting. Even worse, there seems to be no way to reasonably bound the difference of the two sides.

The lack of the chain rule on graphs is the main difficulty in trying to prove a discrete analogue of (1.1). In general on graphs, the fact that the chain rule fails causes major problems. See also [**2**, **7**, **8**, **9**] for other attempts to avoid or partially bypass the chain rule in the discrete setting. In what follows we explain our solution to this issue. First, we consider a one-parameter family of simple identities on manifolds which resembles (1.2) (see also [**27**]): For every $p > 0$ one has

$$\Delta u^p = pu^{p-1}\Delta u + \frac{p-1}{p} u^{-p}|\nabla u^p|^2. \tag{1.3}$$

These also follow from the chain rule. Then, we make the following crucial observation: While there exists no chain rule in the discrete setting, quite remarkably, identity (1.3) for $p = 1/2$ still holds on graphs. This fact is the starting point and probably the most important observation of this paper.

Naively, this means that each time identity (1.2) is applied in the proof of (1.1) we may try to replace it by identity (1.3) with $p = 1/2$. Indeed, this idea starts our work in this paper. However, this idea alone is not enough to prove a discrete analogue of (1.1): We have to redefine the notion of curvature on graphs as explained in the next section.

1.2. A new notion of curvature for graphs. The second obstacle we have to overcome in proving gradient estimates on graphs is that a proper notion of curvature on graphs is not a priori clear. It is a well-known problem to extend the notion of Ricci curvature, or more precisely to define lower bounds for the Ricci curvature in more general spaces than Riemannian manifolds. At present a lot of research has been done in this direction (see e.g. [**12**, **20**, **21**, **24**, **25**, **28**]). The approach to generalizing curvature in the context of gradient estimates by the use of curvature-dimension inequalities explained below was pioneered by Bakry and Emery [**3**].

On a Riemannian manifold M Bochner's identity reveals a connection between harmonic functions or, more generally, solutions of the heat equation and the Ricci curvature. It is given by

$$\forall f \in C^\infty(M) \quad \frac{1}{2}\Delta|\nabla f|^2 = \langle \nabla f, \nabla \Delta f\rangle + \|\mathrm{Hess} f\|_2^2 + \mathrm{Ric}(\nabla f, \nabla f).$$

An immediate consequence of the Bochner identity is that on an n-dimensional manifold whose Ricci curvature is bounded from below by K one has

$$\frac{1}{2}\Delta|\nabla f|^2 \geq \langle \nabla f, \nabla \Delta f\rangle + \frac{1}{n}(\Delta f)^2 + K|\nabla f|^2, \tag{1.4}$$

which is called the *curvature-dimension inequality* (CD-inequality). It was an important insight by Bakry and Emery [**3**] that one can use it as a substitute for the lower Ricci curvature bound on spaces where a direct generalization of Ricci curvature is not available.

Since all known proofs of the Li-Yau gradient estimate exploit non-negative curvature condition through the CD-inequality (1.4), one would believe it is a natural choice in our case as well. Bakry and Ledoux [**4**] succeed in using it to generalize (1.1) to Markov operators on general measure spaces when the operator satisfies a chain rule type formula.

As we have explained in Section 1.1, there is no chain rule in the discrete setting. However, due to formula (1.3) with $p = 1/2$, which compensates for the lack of the chain rule, we succeed in modifying the standard CD-inequality on graphs in order to define a *new* curvature notion on graphs (cf. §3) which we can use to prove a discrete gradient estimate in Theorem 4.4.

One may argue that as we modify the curvature notion it might not be natural anymore. In fact, we show it is natural in several respects: First, we prove that our modified CD-inequality follows from the classical one in situations where the chain rule does hold (Theorem 3.16). Second, we compute it in several examples (§6) to show it gives reasonable results. In particular, we show that trees can have negative curvature K with $|K|$ arbitrarily large. So far the existing notions of curvature [**20**, **25**] always gave $K \geq -2$ for trees. Third, as mentioned above, we derive polynomial volume growth for graphs satisfying non-negative curvature condition, like on manifolds (Corollary 7.8), and it seems to be a first result of this kind on graphs.

1.3. Background on the parabolic Harnack inequality on graphs. Inequality (1.1) can be integrated over space-time, and some new distance function on space-time can be introduced to measure the ratio of the positive solution at different points:

$$u(x,s) \leq C(x,y,s,t)u(y,t) \ , \tag{1.5}$$

where $C(x,y,s,t)$ depends only on the distance of (x,s) and (y,t) in space-time. Using this, [**19**] also gave a sharp estimate of the heat kernel in terms of such a distance function.

Harnack inequalities like (1.5) have many applications. Besides implying bounds on the heat kernel, they can be used to prove eigenvalue estimates, and it is one of the main techniques in the regularity theory of PDEs. Hence it is important to decide what manifolds satisfy such an inequality. Saloff-Coste [**26**] gave a complete characterization of such manifolds (see also Grigor'yan [**13**] for an interesting alternative proof that the Poincaré inequality in conjunction with volume doubling implies the Harnack inequality). Saloff-Coste showed that satisfying a volume doubling property along with Poincaré inequalities is actually equivalent to satisfying the Harnack inequality (1.5). The characterization by Saloff-Coste generalizes the non-negative Ricci curvature condition by Li and Yau, since it is known by combining the Bishop-Gromov comparison theorem [**5**] and the work of Buser [**6**] that a lower bound on the Ricci curvature implies volume doubling and the Poincaré inequality (see also the paper of Grigor'yan, [**13**]). However, a major drawback of the characterization by Saloff-Coste is that showing that a manifold satisfies these properties is rather difficult as both volume doubling and the Poincaré inequality are global in nature. The results in [**19**] have the advantage that a simple local condition, a lower bound on curvature, is sufficient to guarantee that the more global properties hold, at the cost of being more sensitive to perturbations.

In the case of graphs Delmotte [**10**] proved a characterization analogous to that of Saloff-Coste for both continuous and discrete time. However, just as for manifolds, his conditions are hard to verify because of their global nature. One virtue of our results is that they give *local* conditions that imply Harnack-type inequalities.

Organization of the paper. In Section 2 we set up the scope of this paper. In Section 3 we define our notion of curvature by modifying the standard curvature-dimension inequality, and we study the basic properties of the curvature. In particular, we show that on manifolds the modified CD-inequality follows from the classical one. Our main results are contained in Section 4, where we establish the discrete analogue of the gradient estimate (1.1). In Section 5, we use the gradient estimates to derive Harnack inequalities. Section 6 contains curvature computations for certain classes of graphs. In particular we give a general lower bound for graphs with bounded degree and show that this bound is asymptotically sharp in the case of trees. We also show that lattices, and more generally Ricci-flat graphs in the sense of Chung and

Yau [**7**], have non-negative curvature. Finally, in Section 7 we apply our results to derive heat kernel bounds and polynomial volume growth, and to prove a Buser-type eigenvalue estimate.

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2. Setup and notation

First we fix our notation. Let $G = (V, E)$ be a graph. We allow the edges on the graph to be weighted; that is, the edge xy from x to y has weight $w_{xy} > 0$. We say that the graph is unweighted if $w_{xy} \equiv 1$. We do not require that the edge weights be symmetric, so $w_{xy} \neq w_{yx}$ in general, for the proofs of the main theorems, but our key examples satisfying the curvature condition do have symmetric weights. We do, however, require that

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

Moreover, we assume in the following that the graph is locally finite, i.e. $\deg(x) := \sum_{y\sim x} w_{xy} < \infty$ for all $x \in V$.

Given a measure $\mu : V \to \mathbb{R}$ on V, the μ-Laplacian on G is the operator $\Delta : \mathbb{R}^{|V|} \to \mathbb{R}^{|V|}$ defined by

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

Since such averages will appear numerous times in computations, we introduce an abbreviated notation for "averaged sum": For a vertex $x \in V$,

$$\widetilde{\sum_{y\sim x}} h(y) := \frac{1}{\mu(x)} \sum_{y\sim x} w_{xy} h(y).$$

Given a graph and a measure, we define

$$D_w = \max_{\substack{x,y\in V\\ x\sim y}} \frac{\deg(x)}{w_{xy}}$$

and

$$D_\mu = \max_{x\in V} \frac{\deg(x)}{\mu(x)}.$$

So far as is possible, we will treat μ-Laplacian operators generally. The special cases of most interest, however, are the cases where $\mu \equiv 1$, which is the standard graph Laplacian, and the case where $\mu(x) = \sum_{y\sim x} w_{xy} = \deg(x)$, which yields the normalized graph Laplacian. Throughout the remainder of the paper, we will simply refer to the μ-Laplacian as the Laplacian, except when it is important to emphasize the effect of the measure.

In this paper, we are interested in functions $u : V \times [0,\infty) \to \mathbb{R}$ that are solutions of the heat equation. Let us introduce the operator

$$\mathcal{L} = \Delta - \partial_t.$$

We say that $u(x,t)$ is a positive solution to the heat equation, if $u > 0$ and $\mathcal{L}u = 0$. It is not hard to see that such solutions can be written as $u(x,t) = P_t u_0$ when $u_0 = u(\cdot, 0) \in \ell^p(V,\mu)$ for some $1 \leq p \leq \infty$. Here $P_t = e^{t\Delta}$ is the heat kernel and $\ell^p(V,\mu) = \{f : V \to \mathbb{R} : \sum f(x)^p \mu(x) < \infty\}$. Note that the heat equation of course also depends on the measure μ, through the Laplacian it contains.

3. Curvature-dimension inequalities

In this section we introduce a new version of the CD-inequality, which is one of the key steps in deriving analogues of the Li-Yau gradient estimate. We also compare our new notion to the standard CD-inequality. First we need to recall [**4**] the definition of two natural bilinear forms associated to the Laplacian.

Definition 3.1. The gradient form $\Gamma = \Gamma^\Delta$ is defined by

$$\begin{aligned} 2\Gamma(f,g)(x) &= \big(\Delta(f\cdot g) - f\cdot\Delta(g) - \Delta(f)\cdot g\big)(x) \\ &= \frac{1}{\mu(x)}\sum_{y\sim x} w_{xy}(f(y)-f(x))(g(y)-g(x)). \end{aligned}$$

We write $\Gamma(f) = \Gamma(f,f)$. Similarly, the iterated gradient form $\Gamma_2^\Delta = \Gamma_2$ is defined by

$$2\Gamma_2(f,g) = \Delta\Gamma(f,g) - \Gamma(f,\Delta g) - \Gamma(\Delta f, g).$$

We write $\Gamma_2(f) = \Gamma_2(f,f)$.

Definition 3.2. We say that a graph G satisfies the CD-inequality $CD(n,K)$ if, for any function f,

$$\Gamma_2(f) \geq \frac{1}{n}(\Delta f)^2 + K\Gamma(f).$$

Note that this is exactly the CD-inequality in (1.4) written in the Γ notation. G satisfies $CD(\infty, K)$ if

$$\Gamma_2(f) \geq K\Gamma(f).$$

We shall drop the superscript Δ from the Γ and Γ_2 notation unless it would be confusing.

Remark 3.3. The previous definitions can be applied to a broad class of operators, not just our Δ, and to a broad class of spaces, not just graphs. In fact Bakry and Ledoux [**4**] have shown that in a rather general setting $CD(n,0)$ is sufficient to derive the gradient estimate (1.1) for the semigroup generated by an operator L, as long as it is a diffusion semigroup in the following sense.

Definition 3.4. Given an operator L, the semigroup $P_t = e^{t\cdot L}$ is said to be a *diffusion semigroup* if the following identities are satisfied for any smooth function $\Phi : \mathbb{R} \to \mathbb{R}$.

$$\Gamma^L(f, g\cdot h) = g\cdot\Gamma^L(f,h) + h\cdot\Gamma^L(f,g) \tag{3.5}$$

$$\Gamma^L(\Phi\circ f, g) = \Phi'(f)\Gamma^L(f,g) \tag{3.6}$$

$$L(\Phi\circ f) = \Phi'(f)L(f) + \Phi''(f)\Gamma^L(f) \tag{3.7}$$

The main example of such a semigroup is the one generated by the Laplace-Beltrami operator on a Riemannian manifold.

The Laplacian Δ we are interested in does *not* generate a diffusion semigroup, but remarkably, as we mentioned in the introduction, for the choice of $\Phi(f) = \sqrt{f}$ a key formula similar to a combination of (3.6) and (3.7) still holds:

$$2\sqrt{f}\Delta\sqrt{f} = \Delta f - 2\Gamma(\sqrt{f}). \tag{3.8}$$

This can be viewed as the discrete analogue of (1.3) for $p = 1/2$, and it is a simple consequence of the identity

$$2\sqrt{a}(\sqrt{b}-\sqrt{a}) = (b-a) - (\sqrt{b}-\sqrt{a})^2.$$

We haven't been able to find useful discrete analogues of (1.3) for any other value of p.

The identity (3.8) motivates the following key modification of the CD-inequality.

Definition 3.9. We say that a graph G satisfies the *exponential curvature dimension inequality* at the point $x \in V$, $CDE(x,n,K)$ if for any positive function $f : V \to \mathbb{R}$ such that $(\Delta f)(x) < 0$ we have

$$\Gamma_2(f)(x) - \Gamma\left(f, \frac{\Gamma(f)}{f}\right)(x) \geq \frac{1}{n}(\Delta f)(x)^2 + K\Gamma(f)(x)\ .$$

We say that $CDE(n,K)$ is satisfied if $CDE(x,n,K)$ is satisfied for all $x \in V$.

Remark 3.10. For convenience, we set

$$\widetilde{\Gamma}_2(f) := \Gamma_2(f) - \Gamma\left(f, \frac{\Gamma(f)}{f}\right), \tag{3.11}$$

or equivalently by (3.8),

$$\widetilde{\Gamma}_2(f) = \frac{1}{2}\Delta\Gamma(f) - \Gamma\left(f, \frac{\Delta(f^2)}{2f}\right). \tag{3.12}$$

Remark 3.13. An important aspect of both $CD(n, K)$ and CDE (n, K) is that they are local properties: satisfying $CD(n, K)$ or $CDE(n, K)$ at any given vertex depends only on its radius 2 neighborhood. Thus, in principle, it is possible to classify all (unweighted) graphs which satisfy $CDE(n, K)$ and have maximum degree at most D for any fixed D.

Of course, one hopes that typical graphs which one might consider to have non-negative curvature satisfy $CDE(n, 0)$ for some "dimension" n. As we will show in Section 6, the class of Ricci-flat graphs [**7**], which includes abelian Cayley graphs and most notably the standard lattices $\mathbb{Z}^d$ (along with finite tori), do indeed satisfy $CDE(2d, 0)$.

Remark 3.14. The reason we use the adjective "exponential" in Definition 3.9 is revealed in Lemma 3.15 below.

Lemma 3.15. *If the semigroup generated by L is a diffusion semigroup, then for any positive function f one has*

$$\widetilde{\Gamma}_2(f) = f^2\Gamma_2(\log f).$$

Proof. We compute

$$\begin{aligned}
2\Gamma_2(\log f) =& L\Gamma(\log f) - 2\Gamma(\log f, L\log f)\\
=& L\left(\frac{\Gamma(f)}{f^2}\right) - \frac{2}{f}\Gamma\left(f, \frac{Lf}{f} - \frac{\Gamma(f)}{f^2}\right)\\
=& \frac{L\Gamma(f)}{f^2} + 2\Gamma\left(\frac{1}{f^2}, \Gamma(f)\right) + \Gamma(f)L\left(\frac{1}{f^2}\right)\\
& - \frac{2\Gamma(f, Lf)}{f^2} - \frac{2Lf}{f}\Gamma(f, f^{-1})\\
& + \frac{2}{f^3}\Gamma(f, \Gamma(f)) + \frac{2\Gamma(f)}{f}\Gamma(f, f^{-2})\\
=& \frac{2\Gamma_2(f)}{f^2} - \frac{4}{f^3}\Gamma(f, \Gamma(f)) - 2\Gamma(f)\frac{L(f)}{f^3} + 6\frac{\Gamma(f)^2}{f^4}\\
& + \frac{2}{f^3}Lf\Gamma(f) + \frac{2}{f^3}\Gamma(f, \Gamma(f)) - 4\frac{\Gamma(f)^2}{f^4}
\end{aligned}$$

$$=\frac{2\Gamma_2(f)}{f^2}-\frac{2}{f^3}\Gamma(f,\Gamma(f))+2\frac{\Gamma(f)^2}{f^4}$$
$$=\frac{2\Gamma_2(f)}{f^2}-\frac{2}{f^3}\Gamma(f,\Gamma(f))-2\frac{\Gamma(f)}{f^2}\Gamma(f,f^{-1})$$
$$=\frac{2}{f^2}\left(\Gamma_2(f)-\Gamma\left(f,\frac{\Gamma(f)}{f}\right)\right)=\frac{2\widetilde{\Gamma}_2(f)}{f^2}.$$

q.e.d.

Theorem 3.16. *If the semigroup generated by L is a diffusion semigroup, then the condition $CD(n,K)$ implies $CDE(n,K)$.*

Proof. Let f be a positive function such that $(Lf)(x)<0$. By Lemma 3.15,

$$\widetilde{\Gamma}_2(f)=f^2\Gamma_2(\log f)\geq f^2\left(\frac{1}{n}(L\log f)^2+K\cdot\Gamma(\log f)\right)\tag{3.17}$$
$$=\frac{1}{n}f^2(L\log f)^2+K\Gamma(f)\ .\tag{3.18}$$

On the other hand,

$$f(x)L(\log f)(x)=(Lf)(x)-\frac{\Gamma(f)(x)}{f(x)}\leq(Lf)(x)<0.\tag{3.19}$$

Squaring (3.19) and inserting the result in (3.17) yield

$$\widetilde{\Gamma}_2(f)(x)\geq\frac{1}{n}(Lf)(x)^2+K\Gamma(f)(x)\ .$$

q.e.d.

Remark 3.20. Let us define that a graph satisfies the condition $CDE'(n,K)$ if, for all $f>0$,

$$\widetilde{\Gamma}_2(f)\geq\frac{1}{n}f^2(\Delta\log f)^2+K\Gamma(f).$$

In light of Lemma 3.15 and Theorem 3.16, for diffusion semigroups $CD(n,K)\Leftrightarrow CDE'(n,K)\Rightarrow CDE(n,K)$; thus it is tempting to base our curvature notion on CDE' instead of CDE.

Rather interestingly, making such a definition in the graph case loses something: First, as we show below in Theorem 6.8, the integer grid $\mathbb{Z}^d$ satisfies $CDE(2d,0)$. On the other hand, it only satisfies $CDE'(4.53d,0)$ and this dimension constant essentially cannot be improved. Second, it turns out that some graphs (and, in particular, regular trees) do not satisfy $CDE'(n,-K)$ for any $K>0$. In contrast, we show in Theorem 6.1 below that all graphs satisfy $CDE(2,-K)$ for some $K>0$.

4. Gradient estimates

In this section we prove discrete analogues of the Li-Yau gradient estimate (1.1) for graphs satisfying the CDE-inequality.

4.1. Failure of inequality (1.1) **on graphs.** Let us start by explaining why (1.1) in its original form fails on graphs. Let G be any nontrivial graph and $p, q \in V(G)$ two adjacent vertices. Let $u(x,t)$ be the solution of the heat equation with initial condition $u(x,0) = \delta_p$. It is well known that in this case $u(x,t)$ is the distribution at time t of the continuous time simple random walk started at p. The continuous time random walk is obtained by having the walker iterate the following action: Wait for a random time according to an exponential distribution and then take a random step. Let E_1, E_2 be the exponential random variables used in waiting to take the first two steps. Then for small t we have

$$\begin{array}{rcccl} u(p,t) & \geq & P(E_1 > t) = 1 - \int_0^t e^{-s} ds & \geq & 1 - t, \\ u(q,t) & \leq & P(E_1 < t) & \leq & t, \\ u(q,t) & \geq & \frac{1}{\deg(p)} P(E_1 < t) P(E_2 > t) & \geq & \frac{t(1-t)}{2\deg(p)}. \end{array}$$

Thus

$$\frac{|\nabla u|^2(q,t)}{u(q,t)^2} \geq \frac{(1-2t)^2}{t^2} > \frac{1}{2t^2} \ .$$

On the other hand, $\exists t_0 > 0$ small such that $(\partial_t u)(q, t_0) \leq 1$. We conclude that

$$\frac{\partial_t u}{u}(q, t_0) \leq \frac{2\deg(p)}{t_0(1-t_0)} \leq \frac{4\deg(p)}{t_0} \ .$$

The two terms together are still too big:

$$\frac{|\nabla u|^2(q,t_0)}{u(q,t_0)^2} - \frac{\partial_t u}{u}(q,t_0) \geq \frac{1}{2t_0^2} - \frac{4\deg(p)}{t_0} > \frac{n}{2t_0}.$$

Remark 4.1. There is a one-parameter family of possible gradient estimates:

$$\mathcal{E}_p : \frac{|\nabla u^p|^2}{u^{2p}} - \frac{\partial_t u}{u} \leq \frac{n}{2t}.$$

Since in the Riemannian case $\frac{|\nabla u^p|^2}{u^{2p}} = p\frac{|\nabla u|^2}{u^2}$, the original Li-Yau inequality corresponds to $\mathcal{E}_1$, and the larger p is, the stronger $\mathcal{E}_p$ is.

The argument preceding the remark in fact shows that $\mathcal{E}_p$ cannot hold for any graph for any $p > 0.5$. The inequalities we obtain in the sequel are for exactly $p = 0.5$ which, in this sense, is the best exponent one can hope for in discrete Li-Yau gradient estimates.

4.2. Preliminaries. The following lemma, describing the behavior of a function near its local maximum, will be used repeatedly throughout the whole section.

Lemma 4.2. *Let $G(V,E)$ be a (finite or infinite) graph, and let $g, F : V \times [0,T] \to \mathbb{R}$ be functions. Suppose that $g \geq 0$, and F has a local maximum at $(x^*, t^*) \in V \times [0,T]$. Then*

$$\mathcal{L}(gF)(x^*,t^*) \leq (\mathcal{L}g)F(x^*,t^*).$$

Proof. On the one hand,

$$\begin{aligned}\Delta(gF)(x^*,t^*) &= \frac{1}{\mu(x^*)}\sum_{y\sim x^*} w_{x^*y}(g(y,t^*)F(y,t^*) - g(x^*,t^*)F(x^*,t^*))\\ &\le \frac{1}{\mu(x^*)}\sum_{y\sim x^*} w_{x^*y}(g(y,t^*)F(x^*,t^*) - g(x^*,t^*)F(x^*,t^*))\\ &= (\Delta g)F(x^*,t^*).\end{aligned}$$

On the other hand,

$$\partial_t(gF)(x^*,t^*) = (\partial_t g)F(x^*,t^*) + g(\partial_t F)(x^*,t^*) \ge (\partial_t g)F(x^*,t^*),$$

since $\partial_t F = 0$ at the local maximum if $0 < t^* < T$ and $\partial_t F \ge 0$ if $t^* = T$. The last claim is just the difference of the previous two. q.e.d.

For convenience, we also record here some simple facts which we use repeatedly in our proofs of the gradient estimates.

Lemma 4.3. *Suppose $f : V \to \mathbb{R}$ satisfies $f > 0$, and $(\Delta f)(x) < 0$ at some vertex x. Then*

$$(i) \qquad \max_{y\sim x} \frac{w_{xy}}{\mu(x)} f(y) \le \widetilde{\sum_{y\sim x}} f(y) < D_\mu f(x).$$

$$(ii) \qquad \widetilde{\sum_{y\sim x}} f^2(y) < D_\mu D_w f^2(x).$$

Proof. (i) is obvious as $f > 0$. (ii) follows as

$$\widetilde{\sum_{y\sim x}} f^2(y) \le \frac{\mu(x)}{\min_{y\sim x} w_{xy}} \left(\widetilde{\sum_{y\sim x}} f(y)\right)^2 < D_\mu D_w f^2(x).$$

q.e.d.

4.3. Estimates on finite graphs. We begin by proving the gradient estimate in the compact case without boundary. That is, we prove gradient estimates valid for positive solutions to parabolic equations on finite graphs.

Theorem 4.4. *Let G be a finite graph satisfying $CDE(n,0)$, and let u be a positive solution to the heat equation on G. Then for all $t > 0$,*

$$\frac{\Gamma(\sqrt{u})}{u} - \frac{\partial_t(\sqrt{u})}{\sqrt{u}} \le \frac{n}{2t}\ .$$

Proof. Let

$$F = t\left(\frac{2\Gamma(\sqrt{u})}{u} - \frac{2\partial_t(\sqrt{u})}{\sqrt{u}}\right). \tag{4.5}$$

Fix an arbitrary $T > 0$. Our goal is to show that $F(x,T) \leq n$ for every $x \in V$. Let (x^*, t^*) be a maximum point of F in $V \times [0,T]$. We may assume $F(x^*, t^*) > 0$. Hence $t^* > 0$. Moreover, by identity (3.8), which is true both in the continuous and the discrete setting, we know that

$$F = t\left(\frac{2\Gamma(\sqrt{u})}{u} - \frac{\Delta u}{u}\right) = t \cdot \frac{-2\Delta\sqrt{u}}{\sqrt{u}}\ , \tag{4.6}$$

where we used the fact that $\mathcal{L}u = 0$ (recall that $\mathcal{L} = \Delta - \partial_t$), which implies

$$2\frac{\partial_t\sqrt{u}}{\sqrt{u}} = \frac{\partial_t u}{u} = \frac{\Delta u}{u}. \tag{4.7}$$

We conclude from (4.6) that

$$(\Delta\sqrt{u})(x^*, t^*) < 0. \tag{4.8}$$

In what follows all computations are understood to take place at the point (x^*, t^*). We apply Lemma 4.2 with the choice $g = u$. This gives

$$\begin{aligned}\mathcal{L}(u)\cdot F \geq \mathcal{L}(u\cdot F) &= \mathcal{L}(t^*\cdot(2\Gamma(\sqrt{u}) - \Delta u))\\ &= t^*\cdot\mathcal{L}(2\Gamma(\sqrt{u}) - \Delta u) - (2\Gamma(\sqrt{u}) - \Delta u),\end{aligned}$$

where we used (4.6) and the definition of $\mathcal{L}$. We know that $\mathcal{L}(u) = 0$. Also, since Δ and $\mathcal{L}$ commute, $\mathcal{L}(\Delta u) = 0$. So we are left with

$$\begin{aligned}\frac{uF}{t^*} &= 2\Gamma(\sqrt{u}) - \Delta u \geq t^*\cdot\mathcal{L}(2\Gamma(\sqrt{u}))\\ &= t^*\cdot\big(2\Delta\Gamma(\sqrt{u}) - 4\Gamma(\sqrt{u}, \partial_t\sqrt{u})\big) = 4t^*\cdot\widetilde{\Gamma}_2(\sqrt{u})\ .\end{aligned} \tag{4.9}$$

The last equality is true by (3.12) and (4.7). By (4.8) and the $CDE(n,0)$-inequality applied to $\sqrt{u}(\cdot, t^*)$ we get

$$\frac{uF}{t^*} \geq \frac{4t^*}{n}\left(\Delta(\sqrt{u})\right)^2 \overset{(4.6)}{=} \frac{t^*}{n}\left(-\frac{\sqrt{u}F}{t^*}\right)^2 = \frac{u}{nt^*}F^2.$$

Thus $F \leq n$ at (x^*, t^*) as desired. q.e.d.

We can extend the result to the case of graphs satisfying $CDE(n, -K)$ for some $K > 0$ as follows.

Theorem 4.10. *Let G be a finite graph satisfying $CDE(n, -K)$ for some $K > 0$ and let u be a positive solution to the heat equation on G. Fix $0 < \alpha < 1$. Then for all $t > 0$*

$$\frac{(1-\alpha)\Gamma(\sqrt{u})}{u} - \frac{\partial_t(\sqrt{u})}{\sqrt{u}} \leq \frac{n}{(1-\alpha)2t} + \frac{Kn}{\alpha}.$$

Proof. We proceed similarly to the previous case, so we do not repeat computations that are exactly the same. Let

$$F = t \cdot \frac{2(1-\alpha)\Gamma(\sqrt{u}) - \Delta u}{u} \le t \cdot \frac{-2\Delta\sqrt{u}}{\sqrt{u}}.$$

Fix an arbitrary $T > 0$, and we will prove the estimate at (x, T) for all $x \in V$. As before let (x^*, t^*) be the place where F assumes its maximum in the $V \times [0, T]$ domain. We may assume $F(x^*, t^*) > 0$; otherwise there is nothing to prove. Hence $t^* > 0$ and $\Delta\sqrt{u}(x^*, t^*) < 0$.

In what follows all computations are understood at the point (x^*, t^*).

We again apply Lemma 4.2 with the choice $g = u$. As before, this gives

$$0 = \mathcal{L}(u) \cdot F \ge \mathcal{L}(u \cdot F) = \mathcal{L}(t \cdot (2(1-\alpha)\Gamma(\sqrt{u}) - \Delta u)) \\ = 4(1-\alpha)t^* \cdot \widetilde{\Gamma}_2(\sqrt{u}) - \frac{uF}{t^*}.$$

Applying the $CDE(n, -K)$ inequality to $\sqrt{u}$, multiplying by $t^*/((1-\alpha)u)$ and rearranging give

$$\frac{F}{1-\alpha} \ge \frac{4(t^*)^2}{u}\widetilde{\Gamma}_2(\sqrt{u}) \overset{CDE(n,-K)}{\ge} \frac{4(t^*)^2}{u}\left(\frac{1}{n}(2\Delta\sqrt{u})^2 - K\Gamma(\sqrt{u})\right) = \\ = \frac{1}{n}\left(t^*\frac{2\Delta\sqrt{u}}{\sqrt{u}}\right)^2 - 4(t^*)^2K\Gamma(\sqrt{u})/u.$$

Let us denote $G = t^* \cdot 2\Gamma(\sqrt{u})/u$. Then $F + \alpha G = t^* \frac{-2\Delta\sqrt{u}}{\sqrt{u}}$ so this inequality can be rewritten as

$$\frac{F}{1-\alpha} \ge \frac{1}{n}(F + \alpha G)^2 - 2t^*KG.$$

After expanding $(F + \alpha G)^2$ we throw away the $F \cdot G$ term, and use $\alpha^2 G^2$ to bound the last term on the right hand side as follows. Completing the quadratic and linear term in G to a perfect square yields

$$\alpha^2G^2 - 2t^*KnG \ge -\left(\frac{t^*Kn}{\alpha}\right)^2 = -(t^*)^2C(\alpha, n, K). \tag{4.11}$$

So we have $F^2 \le nF/(1-\alpha) + t^2C$, which implies

$$F(x, T) \le F(x^*, t^*) \le \frac{n}{1-\alpha} + t^*\sqrt{C} \le \frac{n}{1-\alpha} + T\frac{Kn}{\alpha},$$

which proves the gradient estimate at (x, T) for all $x \in V$. Since T is arbitrary, we have the theorem as claimed. q.e.d.

We can also extend the result from solutions to the more general operator $(\mathcal{L} - q) = (\Delta - \partial_t - q)u = 0$, where $q(x, t)$ is a potential satisfying $\Delta q \le \vartheta$ and $\Gamma(q) \le \eta^2$ for some $\vartheta \ge 0$ and $\eta \ge 0$.

Theorem 4.12. *Let G be a finite graph and $q(x,t) : V \times \mathbb{R}^+ \to \mathbb{R}$ be a potential satisfying $\Delta q \leq \vartheta$ and $\Gamma(q) \leq \eta^2$ for all $x \in V$ and $t \geq 0$. Suppose $u = u(x,t)$ satisfies $(\mathcal{L} - q)u = 0$ on G.*

1) *If G satisfies $CDE(n, 0)$, then for all $t > 0$,*

$$\frac{\Gamma(\sqrt{u})}{u} - \frac{\partial_t(\sqrt{u})}{\sqrt{u}} - \frac{q}{2} < \frac{n}{2t} + \frac{1}{2}\sqrt{n(\vartheta + \eta\sqrt{2D_\mu\,(D_w+1)})}.$$

2) *Fix $0 < \alpha < 1$, and $0 < \epsilon < 1$. If G satisfies $CDE(n, -K)$, for some $K \geq 0$, then for all $t > 0$,*

$$(1-\alpha)\frac{\Gamma(\sqrt{u})}{u} - \frac{\partial_t(\sqrt{u})}{\sqrt{u}} - \frac{q}{2} < \frac{n}{2(1-\alpha)t} + \frac{1}{2}C(\alpha, K, n, \vartheta, \eta, \epsilon),$$

where

$$C(\alpha, n, K, \vartheta, \eta, \epsilon) \;=\; \sqrt{\frac{n}{1-\alpha}\vartheta + \frac{K^2 n^2}{(1-\epsilon)\alpha^2} + \left(\frac{n(1+\alpha D_w)\eta}{(1-\alpha)\alpha^{1/2}\epsilon^{1/4}}\right)^{\frac{4}{3}}}.$$

Proof. Again, the proof is quite similar to the proof of Theorem 4.4 so we do not repeat computations that are exactly the same. Let

$$F = t \cdot \left(\frac{2\Gamma(\sqrt{u}) - u_t}{u} - q\right).$$

As $(\Delta - \partial_t - q)u = 0$, note $u_t = \Delta u - qu$, so we may rewrite F as

$$F = t \cdot \frac{2\Gamma(\sqrt{u}) - \Delta u}{u} = -t \cdot \frac{2\Delta\sqrt{u}}{\sqrt{u}}$$

as before.

Again, we fix an arbitrary T and take (x^*, t^*) to be the place where F assumes its maximum in the $V \times [0, T]$ domain, and we may assume that $F(x^*, t^*) > 0$ and hence $t^* > 0$ and $\Delta\sqrt{u}(x^*, t^*) < 0$. All computations below should be understood at the point (x^*, t^*).

We again apply Lemma 4.2 with the choice $g = u$. The primary difference is that now at the maximum

$$\mathcal{L}(uF) \leq \mathcal{L}(u)F = qu = -2t^* q\sqrt{u}\Delta\sqrt{u}.$$

Then, similarly as before,

(4.13)

$$\begin{aligned} -2t^* q\sqrt{u}\Delta\sqrt{u} &\geq \mathcal{L}(uF) \\ &= -\frac{uF}{t^*} + t^*\left(2\left[\Delta(\Gamma(\sqrt{u})) - 2\Gamma(\sqrt{u}, \frac{u_t}{2\sqrt{u}})\right] - \Delta\mathcal{L}(u)\right) \\ &= -\frac{uF}{t^*} + t^*\left(4\widetilde{\Gamma}_2(\sqrt{u}) + 2\Gamma(\sqrt{u}, q\sqrt{u}) - \Delta(qu)\right). \end{aligned} \tag{4.14}$$

Rearranging (4.14),

(4.15)
$$0 \geq -\frac{uF}{t^*} + t^*\left(4\widetilde{\Gamma}_2(\sqrt{u}) + 2\Gamma(\sqrt{u}, q\sqrt{u}) + 2q\sqrt{u}\Delta\sqrt{u} - \Delta(qu).\right)$$

Note

$$\begin{aligned}\Delta(qu) &= q\sqrt{u}\Delta\sqrt{u} + \sqrt{u}\Delta(q\sqrt{u}) + 2\Gamma(\sqrt{u}, q\sqrt{u}) \\ &= 2q\sqrt{u}\Delta\sqrt{u} + u\Delta q + 2\sqrt{u}\Gamma(\sqrt{u}, q) + 2\Gamma(\sqrt{u}, q\sqrt{u}). \qquad (4.16)\end{aligned}$$

Combining (4.15) and (4.16), we obtain

$$0 \geq -\frac{uF}{t^*} + t^*\left(4\widetilde{\Gamma}_2(\sqrt{u}) - u\Delta q - 2\sqrt{u}\Gamma(\sqrt{u}, q)\right). \qquad (4.17)$$

Finally, we bound

$$2\Gamma(\sqrt{u}, q) \leq \sqrt{2\Gamma(\sqrt{u})2\Gamma(q)} < \eta\sqrt{2D_\mu\left(D_w + 1\right)u}.$$

Here the first inequality follows from an application of Cauchy-Schwarz. The bound on $\Gamma(\sqrt{u})(x^*, t^*)$ follows as $\Delta\sqrt{u}(x^*, t^*) < 0$, and applying Lemma 4.3 (ii) yields

$$\begin{aligned}2\Gamma(\sqrt{u})(x^*, t^*) &= \widetilde{\sum_{y\sim x^*}}(\sqrt{u}(y, t^*) - \sqrt{u}(x^*, t^*))^2 \\ &\leq \widetilde{\sum_{y\sim x^*}}[u(y, t^*) + u(x^*, t^*)] \\ &< D_\mu\left(D_w + 1\right)u(x^*, t^*).\end{aligned}$$

With this, (4.17) gives

$$0 > -\frac{uF}{t^*} + t^*\left(4\widetilde{\Gamma}_2(\sqrt{u}) - u\vartheta - \eta u\sqrt{2D_\mu\left(D_w + 1\right)}\right).$$

Applying the $CDE(n, 0)$ inequality, multiplying by nt^*/u, and rearranging yield

$$F^2 < nF - (t^*)^2 n\left(\vartheta + \eta\sqrt{2D_\mu\left(D_w + 1\right)}\right),$$

which yields the first claim of the theorem, as above.

The general case with negative curvature works by combining the above with the method of Theorem 4.10. In order to get the best constant, a bit of additional care is needed, however.

In the general case,

$$F = t\left(\frac{2(1-\alpha)\Gamma(\sqrt{u}) - u_t}{u} - q\right) = t\left(\frac{-2(1-\alpha)\sqrt{u}\Delta\sqrt{u} - \alpha\Delta u}{u}\right).$$

Following the previous computation, again at (x^*, t^*) maximizing F,

$$\begin{aligned}
&-2(1-\alpha)t^* q\sqrt{u}\Delta\sqrt{u} - \alpha q\Delta u \geq \mathcal{L}(uF)\\
&= -\frac{uF}{t^*} + t^*\left(2(1-\alpha)\left[\Delta(\Gamma(\sqrt{u})) - 2\Gamma(\sqrt{u}, \frac{u_t}{2\sqrt{u}})\right] - \Delta\mathcal{L}(u)\right)\\
&= -\frac{uF}{t^*} + t^*\left(4(1-\alpha)\widetilde{\Gamma}_2(\sqrt{u}) + 2(1-\alpha)\Gamma(\sqrt{u}, q\sqrt{u}) - \Delta(qu)\right).
\end{aligned}$$

After some computation and rearrangement, we get that

$$\begin{aligned}
0 >& -\frac{uF}{t^*} + t^*\Big(4(1-\alpha)\widetilde{\Gamma}_2(\sqrt{u}) -\\
&- (1-\alpha)u\vartheta + 2\sqrt{u}\Gamma(\sqrt{u}, q) + \alpha(q\Delta u - \Delta(qu))\Big)\\
=& -\frac{uF}{t^*} + t^*\Big(4(1-\alpha)\widetilde{\Gamma}_2(\sqrt{u}) -\\
&- (1-\alpha)u\vartheta + 2(1-\alpha)\sqrt{u}\Gamma(\sqrt{u}, q) - \alpha(u\Delta q + 2\Gamma(u,q))\Big).
\end{aligned} \tag{4.18}$$

We handle the $\Gamma(\sqrt{u}, q)$ term slightly differently here, simply applying Cauchy-Schwarz to observe

$$\Gamma(\sqrt{u}, q) \leq \sqrt{\Gamma(\sqrt{u})\Gamma(q)} \leq 2\eta\sqrt{\Gamma(\sqrt{u})}.$$

We similarly apply Cauchy-Schwarz to bound

$$2\Gamma(u,q) \leq 2\sqrt{\Gamma(u)\Gamma(q)} < \eta u\sqrt{\Gamma(u)}.$$

Lemma 4.3 and the fact that $\Delta\sqrt{u}(x^*) < 0$ imply that $\sqrt{u}(y) < D_w\sqrt{u}(x^*)$ for any $y \sim x^*$. Combining these facts, we observe

$$\begin{aligned}
2\Gamma(u) &= u^2(x^*)\widetilde{\sum_{y\sim x^*}}\left(1 - \frac{u(y)}{u(x)}\right)^2\\
&= u^2(x^*)\widetilde{\sum_{y\sim x^*}}\left(1 - \frac{\sqrt{u(y)}}{u(x^*)}\right)\left(1 + \frac{\sqrt{u(y)}}{\sqrt{u(x^*)}}\right)\\
&< 2(D_w+1)^2 u(x^*)\Gamma(\sqrt{u}).
\end{aligned} \tag{4.19}$$

This establishes that

$$(u\Delta q + 2\Gamma(u,q)) < u\vartheta + 2(D_w+1)\eta\sqrt{u\Gamma(\sqrt{u})}.$$

Following the computations of the proof of Theorem 4.10 from (4.11), with the choice of $G = t^* \cdot 2\Gamma(\sqrt{u})/u$, applying the $CDE(n, -K)$ inequality, and multiplying through by t^*/u, we obtain from (4.18) the following:

$$\begin{aligned}
0 > -F + \frac{(1-\alpha)}{n}(F+\alpha G)^2 - 2(1-\alpha)t^* KG&\\
- (\sqrt{2}\eta(1+\alpha D_w))(t^*)^{3/2}\sqrt{G} - (t^*)^2\alpha\theta&
\end{aligned}$$

Multiplying out, ignoring the positive FG term, and further multiplying the result by $\frac{n}{1-\alpha}$, we obtain

$$0 > \frac{-Fn}{1-\alpha} + F^2 + \alpha^2 G^2 - 2t^* KnG - \sqrt{2}\eta(1+\alpha D_w)(t^*)^{3/2}\sqrt{G} - (t^*)^2 \frac{n\theta}{1-\alpha}.$$

A quartic in G arises, and for any $\epsilon \in (0,1)$ we can write this quartic as

$$\begin{aligned}\left((1-\epsilon)\alpha^2 G^2 - 2t^* KnG\right) + \left(\epsilon\alpha^2 G^2 - \sqrt{2}\eta(1+\alpha D_w)(t^*)^{3/2}\sqrt{G}\right) \\ > -(t^*)^2 \left(\frac{(1-\alpha)K^2 n^2}{\epsilon} + \left(\frac{\eta(1+\alpha D_w)}{\epsilon^{1/4}\alpha^{1/2}(1-\alpha)}\right)^{4/3}\right).\end{aligned}$$

In all, we obtain that for any $\epsilon \in (0,1)$,

$$\frac{Fn}{1-\alpha} > F^2 - (t^*)^2 C^2(\alpha, n, K, \vartheta, \eta, \epsilon)$$

where

$$C(\alpha, n, K, \vartheta, \eta, \epsilon) = \sqrt{\frac{n}{1-\alpha}\vartheta + \frac{K^2 n^2}{(1-\epsilon)\alpha^2} + \left(\frac{n(1+\alpha D_w)\eta}{(1-\alpha)\alpha^{1/2}\epsilon^{1/4}}\right)^{\frac{4}{3}}},$$

thus completing the result.

Again, we prove the result for all (x, T) but, as T is arbitrary, this completes the proof of the theorem. q.e.d.

4.4. General estimates in a ball. We can prove somewhat weaker results in the presence of a boundary. We do not assume finiteness of the graph anymore, and we only assume the heat equation is satisfied in a finite ball. Our estimates will depend on the radius of this ball.

We shall prove two types of estimates. In this section we prove the first type that works for any non-negatively curved graph, while the second type requires the existence of a so-called strong cut-off function on the graph that we will discuss later in Section 4.5.

Theorem 4.20. *Let $G(V,E)$ be a (finite or infinite) graph and $R > 0$, and fix $x_0 \in V$.*

1) *Let $u : V \times \mathbb{R} \to \mathbb{R}$ be a positive function such that $\mathcal{L}u(x,t) = 0$ if $d(x, x_0) \leq 2R$. If G satisfies $CDE(n, 0)$ then for all $t > 0$,*

$$\frac{\Gamma(\sqrt{u})}{u} - \frac{\partial_t \sqrt{u}}{\sqrt{u}} < \frac{n}{2t} + \frac{n(1+D_w)D_\mu}{R}$$

in the ball of radius R around x_0.

2) *Let $u : V \times \mathbb{R} \to \mathbb{R}$ be a positive function such that $(\mathcal{L}-q)u(x,t) = 0$ if $d(x, x_0) \leq 2R$, for some function $q(x,t)$ so that $\Delta q \leq \vartheta$ and $\Gamma(q) \leq \eta^2$. If G satisfies $CDE(n, -K)$ for some $K > 0$, then for*

any $0 < \alpha < 1$*, any* $0 < \epsilon < 1$*, and all* $t > 0$*,*

$$\frac{(1-\alpha)\Gamma(\sqrt{u})}{u} - \frac{\partial_t \sqrt{u}}{\sqrt{u}} - \frac{q}{2} < \frac{n}{(1-\alpha)2t} + \frac{n(2+D_w)D_\mu}{(1-\alpha)R} + \frac{1}{2}C(\alpha, n, K, \vartheta, \eta, \epsilon),$$

where

$$C(\alpha, n, K, \vartheta, \eta, \epsilon) = \left(\frac{K^2 n^2}{\alpha^2} + \frac{n}{1-\alpha} \left(\vartheta\eta \left[(1-\alpha)\sqrt{2D_\mu (D_w + 1)} + \alpha\sqrt{2D_\mu (D_w^3 + 1)} \right] \right) \right)^{1/2}$$

in the ball of radius R *around* x_0*.*

Proof. First we consider the non-negative curvature case. Let us define a cut-off function $\phi : V \to \mathbb{R}$ as

$$\phi(v) = \begin{cases} 0 & : \ d(v, x_0) > 2R \\ \frac{2R - d(v,x_0)}{R} & : \ 2R \geq d(v, x_0) \geq R \\ 1 & : \ R > d(v, x_0) \end{cases}$$

We are going to use the maximum principle as in the proof of Theorem 4.4. Let

$$F = t\phi \cdot \frac{2\Gamma(\sqrt{u}) - \Delta u}{u} = t\phi \cdot \frac{-2\Delta\sqrt{u}}{\sqrt{u}},$$

and let (x^*, t^*) be the place where F attains its maximum in $V \times [0, T]$ for some arbitrary but fixed T. Our goal is to prove a bound on $F(x, T)$ for all $x \in V$ and as T is arbitrary this completes the proof. This bound is positive, so we may assume that $F(x^*, t^*) > 0$. In particular this implies that $t^* > 0$, $\phi(x^*) > 0$, and $\Delta\sqrt{u}(x^*, t^*) < 0$.

Let us first assume that $\phi(x^*) = 1/R$. Since positivity of u implies that for any vertex x

$$\frac{-\Delta\sqrt{u}}{\sqrt{u}}(x) = \widetilde{\sum_{y \sim x}} \left(1 - \frac{\sqrt{u}(y)}{\sqrt{u}(x)} \right) \leq \frac{\deg(x)}{\mu(x)} \leq D_\mu,$$

we see that in this case $F(x^*, t^*) \leq 2t^* D_\mu / R$ and thus

$$F(x, T) \leq F(x^*, t^*) \leq 2t^* D_\mu / R \leq \frac{2TD_\mu}{R}.$$

For $x \in B(x_0, R)$, $\phi \equiv 1$, so

$$F(x, T) = T \cdot \frac{\Gamma(\sqrt{u}) - \Delta u}{u}(x, T) \leq \frac{2TD_\mu}{R},$$

and dividing by T yields a stronger result than desired. We may therefore assume that $\phi(x^*) \geq \frac{2}{R}$ and ϕ does not vanish in the neighborhood of x^*.

Now we apply Lemma 4.2 with the choice $F = u/\phi$. Thus we get

$$\mathcal{L}\left(\frac{u}{\phi}\right) F \geq \mathcal{L}\left(\frac{u}{\phi} F\right) = -\frac{uF}{t^*\phi} + t^* \cdot \mathcal{L}(2\Gamma(\sqrt{u}) - \Delta u).$$

Using the fact that $\mathcal{L}(u) = 0$ we can write

$$\mathcal{L}\left(\frac{u}{\phi}\right) = \widetilde{\sum_{y\sim x^*}} \left(\frac{1}{\phi(y)} - \frac{1}{\phi(x^*)}\right) u(y).$$

Using the same computation as in (4.9) we get

$$t^* \cdot \mathcal{L}(2\Gamma(\sqrt{u}) - \Delta u) = 4t^* \widetilde{\Gamma}_2(\sqrt{u}) \geq \frac{t^*}{n}(-2\Delta\sqrt{u})^2 = \frac{t^*}{n}\left(\frac{\sqrt{u}F}{t^*\phi}\right)^2.$$

Putting these together and multiplying through by $t^*\phi^2/u$ we get

$$\phi(x^*)^2 t^* F \cdot \widetilde{\sum_{y\sim x^*}} \left(\frac{1}{\phi(y)} - \frac{1}{\phi(x^*)}\right) \frac{u(y)}{u(x^*)} + \phi F \geq \frac{1}{n} F^2.$$

Let us write $\phi(x^*) = s/R$. Then for any $y \sim x^*$ we have $\phi(y) = (s\pm 1)/R$ or $\phi(y) = s/R$. In any case,

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

Using Lemma 4.3 (ii) we have

$$\begin{aligned}
\phi(x^*)^2 t^* F \cdot & \widetilde{\sum_{y\sim x^*}} \left(\frac{1}{\phi(y)} - \frac{1}{\phi(x^*)}\right) \frac{u(y)}{u(x^*)} \\
&\leq \phi(x^*)^2 t^* F \cdot \widetilde{\sum_{y\sim x^*}} \left|\frac{1}{\phi(y)} - \frac{1}{\phi(x^*)}\right| \frac{u(y)}{u(x^*)} \\
&\leq \frac{2t^* F}{R} \cdot \widetilde{\sum_{y\sim x^*}} \frac{u(y)}{u(x^*)} \\
&< \frac{2t^* D_\mu D_w}{R} F.
\end{aligned}$$

Combining everything, we can see that for any x such that $d(x, x_0) \leq R$ and thus $\phi(x) = 1$, at time T

$$\begin{aligned}
T \cdot \frac{2\Gamma(\sqrt{u}) - \Delta u}{u} &= F(x, T) \leq F(x^*, t^*) \\
&< n \cdot \phi + \frac{2nt^* \deg^2(x^*)}{R\mu(x) w_{\min}} \leq n + \frac{2nT D_w D_\mu}{R},
\end{aligned}$$

and dividing by T gives the result.

The proof of the general case is simply the combination of the preceding proof with that of Theorem 4.12. q.e.d.

Corollary 4.21. If $G(V,E)$ is an infinite, bounded degree graph satisfying $CDE(n,0)$ and u is a positive solution to the heat equation on G, then

$$\frac{\Gamma(\sqrt{u})}{u} - \frac{\partial_t \sqrt{u}}{\sqrt{u}} \leq \frac{n}{2t}$$

on the whole graph.

4.5. Strong cut-off functions. In the case of manifolds [**19**], a result similar to Theorem 4.20 holds with $1/R^2$ instead of $1/R$. In one of the key steps of the argument, the Laplacian comparison theorem is applied to the distance function. This together with the chain rule implies that one can find a cut-off function ϕ that satisfies

$$\Delta\phi \geq -c(n)\frac{1+R\sqrt{K}}{R^2},$$

where c is a constant that only depends on the dimension. Since the cut-off function ϕ also satisfies

$$\frac{|\nabla\phi|^2}{\phi} < \frac{c(n)}{R^2} \tag{4.22}$$

it follows that there exists a constant $C(n)$ that only depends on the dimension such that

$$\Delta\phi - 2\frac{|\nabla\phi|^2}{\phi} \geq -C(n)\frac{1+R\sqrt{K}}{R^2}. \tag{4.23}$$

Unfortunately on graphs the Laplacian comparison theorem for the usual graph distance is not true—think for instance of the lattice $\mathbb{Z}^2$. This is the reason why in general we have to assume the existence of a cut-off function that has similar properties to (4.22) and (4.23), in order to prove a gradient estimate with $1/R^2$. Noting that for a diffusion semigroup and hence in particular for the Laplace-Beltrami operator on manifolds

$$\phi^2\Delta\frac{1}{\phi} = -\Delta\phi + 2\frac{\Gamma(\phi)}{\phi} \leq C(n)\frac{1+R\sqrt{K}}{R^2}$$

and

$$\phi^3\Gamma\left(\frac{1}{\phi}\right) = \frac{\Gamma(\phi)}{\phi} \leq \frac{C(n)}{R^2}$$

this discussion motivates the following definition:

Definition 4.24. Let $G(V,E)$ be a graph satisfying $CDE(n,-K)$ for some $K \geq 0$. We say that the function $\phi : V \to [0,1]$ is a (c,R)-*strong* cut-off function centered at $x_0 \in V$ and supported on a set $S \subset V$ if $\phi(x_0) = 1$, $\phi(x) = 0$ if $x \notin S$, and for any vertex $x \in S$

1) either $\phi(x) < \frac{c(1+R\sqrt{K})}{2R^2}$,

2) or ϕ does not vanish in the immediate neighborhood of x and

$$\phi^2(x)\Delta\frac{1}{\phi}(x) < D_\mu\frac{c(1+R\sqrt{K})}{R^2} \text{ and } \phi^3(x)\Gamma\left(\frac{1}{\phi}\right)(x) < D_\mu\frac{c}{R^2},$$

where the constant $c = c(n)$ only depends on the dimension n.

Remark 4.25. The 'strength' of the strong cut-off function depends on the size of support S. In order to get results akin to those in the manifold case, with $\frac{1}{R^2}$ appearing for solutions valid in $B(x_0, cR)$, one requires a strong cut-off function whose support lies within a ball of radius cR. The cut-off function defined above, using graph distance, gives a strong cut-off function on the ball of radius R^2. Theorem 4.26 yields a better estimate than Theorem 4.20 whenever one can find a strong cut-off function with support in a ball of radius $\ll R^2$.

In Section 6 we will show (see Corollary 6.10 and Proposition 6.14) that the usual Cayley graph of $\mathbb{Z}^d$ with the regular or the normalized Laplacian satisfies $CDE(2d, 0)$ and admits a $(100, R)$-strong cut-off function supported on a ball of radius $\sqrt{d}R$ centered at x_0.

Theorem 4.26. *Let $G(V,E)$ be a (finite or infinite) graph satisfying $CDE(n, -K)$ for some $K \geq 0$. Let $R > 0$ and fix $x_0 \in V$. Assume that G has a (c,R)-strong cut-off function supported on $S \subset V$ and centered at x_0. Fix $0 < \alpha < 1$. Let $u : V \times \mathbb{R} \to \mathbb{R}$ be a positive function such that $(\mathcal{L} - q)u(x,t) = 0$ if $x \in S$, for some $q(x,t)$ satisfying $\Delta q \leq \vartheta$ and $\Gamma(q) \leq \eta^2$. Then for every $\epsilon \in (0,1)$,*

$$\left(\frac{(1-\alpha)\Gamma(\sqrt{u})}{u} - \frac{\partial_t\sqrt{u}}{\sqrt{u}} - \frac{q}{2}\right)(x_0,t) < \frac{n}{2(1-\alpha)t} + \frac{D_\mu cn}{2(1-\alpha)R^2}\left(1 + R\sqrt{K} + \frac{n(D_w+1)^2}{4\alpha(1-\alpha)}\right) + \frac{1}{2}C(\alpha,n,K,\vartheta,\eta,\epsilon),$$

where

$$C(\alpha,n,K,\vartheta,\eta,\epsilon) = \sqrt{\frac{n}{1-\alpha}\vartheta + \frac{K^2n^2}{(1-\epsilon)\alpha^2} + \left(\frac{n(1+\alpha D_w)\eta}{(1-\alpha)\alpha^{1/2}\epsilon^{1/4}}\right)^{\frac{4}{3}}}.$$

As we noted in the remark above, the lattice $\mathbb{Z}^d$ yields a (c,R)-strong cut-off function in the ball $B(x_0, \sqrt{d}R)$ and $CDE(0, 2d)$. As a result Theorem 4.26 specializes to the following.

Corollary 4.27. If u is a solution of the heat equation $\mathcal{L}u = 0$ in $B(x_0, \sqrt{d}R) \subset \mathbb{Z}^d$, then (with the choice $\alpha = 1/2$):

$$\frac{\Gamma(\sqrt{u}) - \Delta u}{u}(x_0,t) \leq \frac{4d}{t} + \frac{c(d)}{R^2}$$

for some explicit constant $c(d)$ depending on the dimension.

Proof of Theorem 4.26. We proceed similarly to the proof of Theorem 4.20, except that we assume ϕ is a (c,R)-strong cut-off function centered at x_0. Let us choose

$$F = t\phi \cdot \frac{2(1-\alpha)\Gamma(\sqrt{u}) - \Delta u}{u},$$

and let (x^*, t^*) denote the place where F attains its maximum in $V \times [0,T]$ for some arbitrary but fixed T. Again, our goal is to show that $F(x,T)$ is bounded for all $x \in V$, and since T is arbitrary this completes the result. We bound F by some positive quantity; hence we may assume $F(x^*,t^*) > 0$. This implies $t^* > 0, \phi(x^*) > 0$, and $2\Gamma(\sqrt{u}) - \Delta u \geq 2(1-\alpha)\Gamma(\sqrt{u}) - \Delta u > 0$ at (x^*,t^*). Hence $\Delta\sqrt{u}(x^*,t^*) < 0$ as in the proof of Theorem 4.20.

First, if $\phi(x^*) \leq \frac{c(1+R\sqrt{K})}{2R^2}$ then we are done, since

$$\frac{2(1-\alpha)\Gamma(\sqrt{u}) - \Delta u}{u} \leq \frac{2\Gamma(\sqrt{u}) - \Delta u}{u} = \frac{-2\Delta\sqrt{u}}{\sqrt{u}} \leq 2D_\mu,$$

as we have seen in the proof of Theorem 4.20. Thus we may assume that case 2 of Definition 4.24 holds.

In what follows all equations are to be understood at (x^*,t^*). We use Lemma 4.2 with the choice $F = u/\phi$ to get

(4.28)
$$\begin{aligned}
\mathcal{L}\left(\frac{u}{\phi}\right) F &\geq \mathcal{L}\left(\frac{u}{\phi} F\right) \\
&= -\frac{uF}{t^*\phi} + t^* \cdot \mathcal{L}(2(1-\alpha)\Gamma(\sqrt{u}) - \Delta u) \\
&= -\frac{uF}{t^*\phi} + t^* \cdot \left[(1-\alpha)\mathcal{L}(2\Gamma(\sqrt{u})) - \Delta(qu)\right]
\end{aligned}$$

(4.29)
$$= -\frac{uF}{t^*\phi} + t^* \cdot \left[4(1-\alpha)\widetilde{\Gamma}_2(\sqrt{u}) + 2(1-\alpha)\Gamma(\sqrt{u},\sqrt{u}q) - \Delta(qu)\right].$$

On the left hand side we use Cauchy-Schwarz:

$$\begin{aligned}
\mathcal{L}\left(\frac{u}{\phi}\right) &= \frac{\mathcal{L}(u)}{\phi} + \mathcal{L}\left(\frac{1}{\phi}\right) u + 2\Gamma\left(\frac{1}{\phi}, u\right) \\
&= \frac{qu}{\phi} + u\Delta\frac{1}{\phi} + 2\Gamma\left(\frac{1}{\phi}, u\right) \\
&\leq \frac{qu}{\phi} + u\Delta\frac{1}{\phi} + 2\sqrt{\Gamma\left(\frac{1}{\phi}\right)}\sqrt{\Gamma(u)}, \qquad (4.30)
\end{aligned}$$

since $\mathcal{L}(u) = qu$.

Collecting the q-terms in (4.29) and using (4.30), we observe that they are

$$
\begin{aligned}
& t^* \left[2(1-\alpha)\Gamma(\sqrt{u},\sqrt{u}q) - \Delta(qu)\right] - \frac{qu}{\phi}F \\
& = t^*[(1-\alpha)\left(2\Gamma(\sqrt{u},\sqrt{u}q) - \Delta(qu) - 2q\sqrt{u}\Delta\sqrt{u}\right) \\
& \quad + \alpha\left(q\Delta(u) - \Delta(qu)\right)] \qquad (4.31)\\
& > -ut^*\left(\vartheta + 2(1-\alpha)\eta\frac{\sqrt{\Gamma(\sqrt{u})}}{\sqrt{u}} + 2\alpha\eta\frac{\sqrt{\Gamma(u)}}{u}\right) \\
& \geq -ut^*\left(\vartheta + 2\eta(1+\alpha D_w)\frac{\sqrt{\Gamma(\sqrt{u})}}{\sqrt{u}}\right) \qquad (4.32)
\end{aligned}
$$

In the computation above we used several times Cauchy-Schwarz, (4.16), and the observation that $\Gamma(u)/u^2$ can be controlled by $\Gamma(\sqrt{u})/u$ in the following way: By Lemma 4.3 (i), and the fact that $\Delta\sqrt{u}(x^*) < 0$, we have that $\sqrt{u}(y) < D_w\sqrt{u}(x^*)$ for any $y \sim x^*$. Hence

$$
\begin{aligned}
\frac{2\Gamma(u)}{u^2} &= \widetilde{\sum_{y\sim x^*}}\left(1 - \frac{u(y)}{u(x^*)}\right)^2 = \widetilde{\sum_{y\sim x^*}}\left(1 - \frac{\sqrt{u}(y)}{\sqrt{u}(x^*)}\right)^2\left(1 + \frac{\sqrt{u}(y)}{\sqrt{u}(x^*)}\right)^2 \\
&< (D_w+1)^2\,\frac{2\Gamma(\sqrt{u})}{u}. \qquad (4.33)
\end{aligned}
$$

Combining (4.32) with (4.29) and multiplying by $t^*\phi^2/u$ we get

$$
\begin{aligned}
(4.34)\quad & (t^*)^2\phi^2\left(\vartheta + 2\eta(1+\alpha D_w)\frac{\sqrt{\Gamma(\sqrt{u})}}{\sqrt{u}}\right) + Ft^*\phi^2\Delta\frac{1}{\phi} \\
& + Ft^*\sqrt{2\phi^3\Gamma\left(\frac{1}{\phi}\right)}\sqrt{\phi\frac{2\Gamma(u)}{u^2}} + \phi F \\
& > 4(1-\alpha)\frac{\widetilde{\Gamma}_2(\sqrt{u})}{u}(t^*)^2\phi^2.
\end{aligned}
$$

Let us introduce the notation $G = 2t^*\phi\Gamma(\sqrt{u})/u$. Using (4.33), and that ϕ is a (c,R)-strong cut-off function, we can further estimate the left hand side of (4.34) from above:

$$
\begin{aligned}
& (t^*)^2\phi^2\vartheta + \sqrt{2}\eta(1+\alpha D_w)(t^*\phi)^{\frac{3}{2}}\sqrt{G} + \frac{t^*D_\mu c(1+R\sqrt{K})}{R^2}F + \phi F \\
(4.35)\quad & + \sqrt{2}\,(D_w+1)\left(\frac{t^*D_\mu c}{R^2}\right)^{\frac{1}{2}} F\sqrt{G} > 4(1-\alpha)\frac{\widetilde{\Gamma}_2(\sqrt{u})}{u}(t^*)^2\phi^2.
\end{aligned}
$$

Using that the graph satisfies $CDE(n,-K)$ we can write

$$4(t^*)^2\phi^2\frac{\widetilde{\Gamma}_2(\sqrt{u})}{u} \geq \frac{1}{n}\left(t^*\phi\frac{2\Delta\sqrt{u}}{\sqrt{u}}\right)^2 - 2K(t^*)^2\phi^2\frac{2\Gamma(\sqrt{u})}{u}$$
$$= \frac{(F+\alpha G)^2}{n} - (2t^*\phi)KG.$$

Combining with (4.35) we have

$$\frac{n}{1-\alpha}\left((t^*)^2\phi^2\vartheta + \sqrt{2}\eta(1+\alpha D_w)(t^*\phi)^{\frac{3}{2}}\sqrt{G}\right)$$
$$+\frac{n}{1-\alpha}\left(\frac{t^*D_\mu c(1+R\sqrt{K})}{R^2} + \phi + \sqrt{2}\,(D_w+1)\left(\frac{t^*D_\mu c}{R^2}\right)^{\frac{1}{2}}\sqrt{G}\right)F$$
$$> F^2 + 2\alpha FG + \alpha^2G^2 - 2t^*\phi KnG.$$

Notice that completing the left hand side to a perfect square gives

$$2\alpha GF - \sqrt{2}\,(D_w+1)\frac{n}{(1-\alpha)}\left(\frac{t^*D_\mu c}{R^2}\right)^{\frac{1}{2}}\sqrt{G}F$$
$$\geq -\frac{t^*D_\mu c}{R^2}(D_w+1)^2\frac{n^2}{4\alpha(1-\alpha)^2}F$$

and hence

$$\frac{n}{1-\alpha}\left((t^*)^2\phi^2\vartheta + \sqrt{2}\eta(1+\alpha D_w)(t^*\phi)^{\frac{3}{2}}\sqrt{G}\right)$$
$$+\frac{n}{1-\alpha}\left(\frac{t^*D_\mu c(1+R\sqrt{K})}{R^2} + \phi + (D_w+1)^2\frac{t^*D_\mu cn}{4\alpha(1-\alpha)R^2}\right)F \tag{4.36}$$
$$> F^2 + \alpha^2G^2 - 2t^*\phi KnG. \tag{4.37}$$

Now we consider the terms from (4.37) containing G, namely

$$\alpha^2G^2 - 2t^*\phi KnG - \frac{n}{1-\alpha}\sqrt{2}\eta(1+\alpha aD_w)(t^*\phi)^{\frac{3}{2}}\sqrt{G}.$$

We give a lower bound on these terms. Letting $\tilde{G} = 2\frac{\Gamma(\sqrt{u})}{\sqrt{u}} = G/(t^*\phi)$ we obtain for every $\epsilon \in (0,1)$

$$(t^*\phi)^2\left(\epsilon\alpha^2\tilde{G}^2 + (1-\epsilon)\alpha^2\tilde{G}^2 - 2Kn\tilde{G} - \frac{n}{1-\alpha}\sqrt{2}\eta(1+\alpha D_w)\sqrt{\tilde{G}}\right)$$
$$\geq (t^*\phi)^2\left(\epsilon\alpha^2\tilde{G}^2 - \frac{K^2n^2}{(1-\epsilon)\alpha^2} - \frac{n}{1-\alpha}\sqrt{2}\eta(1+\alpha D_w)\sqrt{\tilde{G}}\right)$$
$$\geq (t^*\phi)^2\left(-\frac{K^2n^2}{(1-\epsilon)\alpha^2} - \left(\frac{n(1+\alpha D_w)\eta}{(1-\alpha)\alpha^{1/2}\epsilon^{1/4}}\right)^{\frac{4}{3}}\right),$$

where the inequalities follow from minimizing the involved square and quartic.

This combined with (4.37) now yields

$$\frac{n}{1-\alpha}\left(\frac{t^* D_\mu c(1+R\sqrt{K})}{R^2}+\phi+(D_w+1)^2\frac{t^* D_\mu cn}{4\alpha(1-\alpha)R^2}\right)F$$
$$+(t^*\phi)^2\left[\frac{n}{1-\alpha}\vartheta+\frac{K^2n^2}{(1-\epsilon)\alpha^2}+\left(\frac{n(1+\alpha D_w)\eta}{(1-\alpha)\alpha^{1/2}\epsilon^{1/4}}\right)^{\frac{4}{3}}\right]\geq F^2,$$

which easily implies

$$F<\frac{n}{1-\alpha}\left(\frac{t^* D_\mu c(1+R\sqrt{K})}{R^2}+\phi+(D_w+1)^2\,\frac{t^* D_\mu cn}{4\alpha(1-\alpha)R^2}\right)$$
$$+t^*\phi C(\alpha,n,K,\vartheta,\eta,\epsilon)$$

where

$$C(\alpha,n,K,\vartheta,\eta,\epsilon)=\sqrt{\frac{n}{1-\alpha}\vartheta+\frac{K^2n^2}{(1-\epsilon)\alpha^2}+\left(\frac{n(1+\alpha D_w)\eta}{(1-\alpha)\alpha^{1/2}\epsilon^{1/4}}\right)^{\frac{4}{3}}}.$$

Using that $\phi\leq 1$, $\phi(x_0)=1$, $t^*\leq T$, and $F(x_0,T)\leq F(x^*,t^*)$, and finally dividing by T, we get the desired upper bound

$$\frac{(1-\alpha)2\Gamma(\sqrt{u})-\Delta u}{u}(x_0,T)$$
$$<\frac{n}{1-\alpha}\left(\frac{D_\mu c(1+R\sqrt{K})}{R^2}+\frac{1}{T}+(D_w+1)^2\,\frac{D_\mu cn}{4\alpha(1-\alpha)R^2}\right)$$
$$+C(\alpha,n,K,\vartheta,\eta,\epsilon).$$

q.e.d.

5. Harnack inequalities

In this section we explain how the gradient estimates can be used to derive Harnack-type inequalities. The proof is based on the method used by Li and Yau in [**19**], though the discrete space does pose some extra difficulties.

In order to state the result in complete generality (in particular, when f is a solution to $(\mathcal{L}-q)f=0$ as opposed to a solution to the heat equation), we need to introduce a discrete analogue of the Agmon distance between two points x and y which are connected in $B(x_0,R)$. For a path $p_0p_1\dots p_k$ define the length of the path to be $\ell(P)=k$. Then in a graph with bounded measure $\mu \leq \mu_{\max}$:

$$\varrho_{q,x_0,R,\mu_{\max},w_{\min},\alpha}(x,y,T_1,T_2) = \inf \Bigg\{ \frac{2\mu_{\max}\ell^2(P)}{w_{\min}(1-\alpha)(T_2-T_1)} + \sum_{i=0}^{k-1} \left(\int_{t_i}^{t_{i+1}} q(x_i,t)dt + \frac{k}{(T_2-T_1)^2} \int_{t_i}^{t_{i+1}} (t-t_i)^2 (q(x_i,t)-q(x_{i+1},t))dt \right) \Bigg\}$$

where the infinum is taken over the set of all paths $P = p_0p_1p_2p_3\dots p_k$ so that $p_0 = x$, $p_k = y$, and having all $p_i \in B(x_0,R)$, and the times $T_1 = t_0, t_1, t_2, \dots, t_k = T_2$ evenly divide the interval $[T_1,T_2]$. In the case when the graph satisfies $CDE(n,0)$ one can set $\alpha = 0$.

Remark 5.1. In the special case where $q \equiv 0$ and $R = \infty$, which will arise when f is a solution to the heat equation on the entire graph, then ϱ simplifies drastically. In particular,

$$\varrho_{\mu_{\max},\alpha,w_{\min}}(x,y,t_1,t_2) = \frac{2\mu_{\max}d(x,y)^2}{(1-\alpha)(T_2-T_1)w_{\min}},$$

where $d(x,y)$ denotes the usual graph distance.

Theorem 5.2. *Let $G(V,E)$ be a graph with measure bound $\mu_{\max}$, and suppose that a function $f : V \times \mathbb{R} \to \mathbb{R}$ satisfies*

$$(1-\alpha)\frac{\Gamma(f)}{f^2}(x,t) - \frac{\partial_t f}{f}(x,t) - q(x,t) \leq \frac{c_1}{t} + c_2$$

whenever $x \in B(x_0,R)$ for $x_0 \in V$ along with some $R \geq 0$, some $0 \leq \alpha < 1$, and positive constants c_1, c_2. Then for $T_1 < T_2$ and $x, y \in V$ we have

$$f(x,T_1) \leq f(y,T_2)\left(\frac{T_2}{T_1}\right)^{c_1} \cdot \exp\left(c_2(T_2-T_1) + \varrho_{q,x_0,R,\mu_{\max},w_{\min},\alpha}(x,y,T_1,T_2)\right).$$

In the case of unweighted graphs, and when dealing with positive solutions to the heat equation everywhere, Theorem 5.2 simplifies greatly.

Corollary 5.3. Suppose $G(V,E)$ is a finite or infinite unweighted graph satisfying $CDE(n,0)$, and $\mu(x) = \deg(x)$ for all vertices $x \in V$. If u is a positive solution to the heat equation on G, then

$$u(x,T_1) \leq u(y,T_2)\left(\frac{T_2}{T_1}\right)^{n} \exp\left(\frac{4Dd(x,y)^2}{T_2-T_1}\right),$$

where D denotes the maximum degree of a vertex in G.

Remark 5.4. Observe that in the application of Theorem 5.2 to prove the corollary, one may take $c_1 = \frac{n}{2}$ (see Theorem 4.12 and Theorem 4.20), but Theorem 5.2 naturally compares $\sqrt{u(x,T_1)}$ to $\sqrt{u(x,T_2)}$. To compare $u(x,T_1)$ to $u(x,T_2)$ requires squaring both sides and introduces a factor of two in the exponent.

Before we give the proof of Theorem 5.2, we need one simple lemma.

Lemma 5.5. *For any $c > 0$ and any functions $\psi, q_1, q_2 : [T_1, T_2] \to \mathbb{R}$, we have*

$$\begin{aligned}
&\min_{s\in[T_1,T_2]} \psi(s) - \frac{1}{c}\int_s^{T_2} \psi^2(t)dt + \int_{T_1}^{s} q_1(t)dt + \int_s^{T_2} q_2(t)dt \\
&\le \frac{c}{T_2 - T_1} + \int_{T_1}^{T_2} q_1(t)dt + \frac{1}{(T_2-T_1)^2}\int_{T_1}^{T_2}(t-T_1)^2(q_2(t)-q_1(t))dt.
\end{aligned}$$

Proof. We bound the minimum by an averaged sum. Let $\phi(t) = \frac{2}{c}(t - T_1)$. Then

$$\begin{aligned}
&\min_{s\in[T_1,T_2]} \psi(s) - \frac{1}{c}\int_s^{T_2} \psi^2(t)dt + \int_{T_1}^{s} q_1(t)dt + \int_s^{T_2} q_2(t)dt \\
\le&\frac{\int_{T_1}^{T_2}\phi(s)\left(\psi(s) - \frac{1}{c}\int_s^{T_2}\psi^2(t)dt + \int_{T_1}^{s} q_1(t)dt + \int_s^{T_2} q_2(t)dt\right)ds}{\int_{T_1}^{T_2}\phi(s)ds} \\
=&\frac{c}{(T_2-T_1)^2}\left(\int_{T_1}^{T_2}\phi(s)\psi(s)ds - \frac{1}{c}\int_{T_1}^{T_2}\psi^2(t)\int_{T_1}^{t}\phi(s)dsdt\right. \\
&\qquad\left. + \int_{T_1}^{T_2} q_1(t)\int_t^{T_2}\phi(s)dsdt + \int_{T_1}^{T_2} q_2(t)\int_{T_1}^{t}\phi(s)dsdt\right) \\
=&\frac{c}{(T_2-T_1)^2}\left[\int_{T_1}^{T_2}\left(2\frac{t-T_1}{c}\psi(t) - \psi^2(t)\left(\frac{t-T_1}{c}\right)^2\right)dt\right. \\
&\qquad\left. + \int_{T_1}^{T_2}\frac{(T_2-T_1)^2-(t-T_1)^2}{c}q_1(t)dt + \int_{T_1}^{T_2}\frac{(t-T_1)^2}{c}q_2(t)dt\right] \\
\le&\ \frac{c}{T_2 - T_1} + \int_{T_1}^{T_2} q_1(t)dt + \frac{1}{(T_2-T_1)^2}\int_{T_1}^{T_2}(t-T_1)^2(q_2(t)-q_1(t))dt
\end{aligned}$$

as we claimed, since $2x - x^2 \le 1$. q.e.d.

With this, we can return to the proof of Theorem 5.2.

Proof of Theorem 5.2. Let us first assume that $x \sim y$. Then for any $s \in [T_1, T_2]$ we can write

$$\log f(x,T_1) - \log f(y,T_2) = \log\frac{f(x,T_1)}{f(x,s)} + \log\frac{f(x,s)}{f(y,s)} + \log\frac{f(y,s)}{f(y,T_2)}$$
$$= -\int_{T_1}^{s} \partial_t \log f(x,t)dt + \log\frac{f(x,s)}{f(y,s)} - \int_{s}^{T_2} \partial_t \log f(y,t)dt.$$

We use the assumption that

$$-\partial_t \log f = -\frac{\partial_t f}{f} \le \frac{c_1}{t} + c_2 - (1-\alpha)\frac{\Gamma(f)}{f^2} + q$$

to deduce

$$\log f(x,T_1) - \log f(y,T_2) \le \int_{T_1}^{T_2} \frac{c_1}{t}$$
$$+ c_2 dt - (1-\alpha)\left(\int_{T_1}^{s} \frac{\Gamma(f)}{f^2}(x,t)dt + \int_{s}^{T_2} \frac{\Gamma(f)}{f^2}(y,t)dt\right) + \log\frac{f(x,s)}{f(y,s)}$$
$$+ \int_{T_1}^{s} q(x,t)dt + \int_{s}^{T_2} q(y,t)dt$$
$$\le c_1 \log\frac{T_2}{T_1} + c_2(T_2 - T_1) - \frac{(1-\alpha)w_{\min}}{2\mu_{\max}} \int_{s}^{T_2} \left|\frac{f(y,t) - f(x,t)}{f(y,t)}\right|^2$$
$$+ \frac{f(x,s) - f(y,s)}{f(y,s)} + \int_{T_1}^{s} q(x,t)dt + \int_{s}^{T_2} q(y,t)dt.$$

In the second step we threw away the $\int_{T_1}^{s}$ term, and used $\Gamma(f)(y,t) \ge \frac{1}{2}w_{\min}(f(y,t) - f(x,t))^2/\mu_{\max}$ as well as the fact that $\log r \le r - 1$ for any $r \in \mathbb{R}$.

We are free to choose the value of s for which the right hand side is minimal. We use Lemma 5.5, with the choice $\psi(t) = f(x,t)/f(y,t) - 1$ and $c = (1-\alpha)w_{\min}/2\mu_{\max}$ along with $q_1(t) = q(x,t)$ and $q_2(t) = q(y,t)$ to get

(5.6)

$$\log f(x,T_1) - \log f(y,T_2)$$
$$\le c_1 \log\frac{T_2}{T_1} + c_2(T_2 - T_1) + \frac{2\mu_{\max}}{(1-\alpha)(T_2 - T_1)w_{\min}}$$

$$+ \int_{T_1}^{T_2} q(x,t)dt + \frac{1}{(T_2 - T_1)^2}\int_{T_1}^{T_2} (t - T_1)^2(q(y,t) - q(x,t))dt. \tag{5.7}$$

To handle the case when x and y are not adjacent, simply let $x = x_0, x_1, \ldots, x_k = y$ denote a path P between x and y entirely within $B(x_0, R)$, and let $T_1 = t_0 < t_1 < \cdots < t_k = T_2$ denote a subdivision of the time interval $[T_1, T_2]$ into k equal parts. For any $0 \leq i \leq k-1$ we can use (5.7) to get

$$\log f(x,T_1) - \log f(y,T_2) = \sum_{i=0}^{k-1} \big[\log f(x_i,t_i) - \log f(x_{i+1},t_{i+1}) \big]$$
$$\leq \sum_{i=0}^{k-1} \left(c_1 \log \frac{t_{i+1}}{t_i} + c_2(t_{i+1}-t_i) + \frac{2\mu_{\max}}{(1-\alpha)\frac{T_2-T_1}{k} w_{\min}} \right)$$
$$+ \sum_{i=0}^{k-1} \left(\int_{t_i}^{t_{i+1}} q(x_i,t)dt + \right.$$
$$\left. + \frac{k}{(T_2-T_1)^2} \int_{t_i}^{t_{i+1}} (t-t_i)^2 (q(x_i,t) - q(x_{i+1},t))dt \right)$$
$$\leq c_1 \log \frac{T_2}{T_1} + c_2(T_2-T_1) + \frac{2k^2 \mu_{\max}}{(1-\alpha)(T_2-T_1)w_{\min}} + \sum_{i=0}^{k-1} \left(\int_{t_i}^{t_{i+1}} q(x_i,t)dt \right.$$
$$\left. + \frac{k}{(T_2-T_1)^2} \int_{t_i}^{t_{i+1}} (t-t_i)^2 (q(x_i,t) - q(x_{i+1},t))dt \right).$$

Minimizing all paths, we have that

$$\log f(x,T_1) - \log f(y,T_2)$$
$$\leq c_1 \log \frac{T_2}{T_1} + c_2(T_2-T_1) + \varrho_{q,x_0,R,\mu_{\max},w_{\min},\alpha}(x,y,T_1,T_2).$$

Hence

$$f(x,T_1) \leq f(y,T_2) \left(\frac{T_2}{T_1}\right)^{c_1}$$
$$\cdot \exp(c_2(T_2-T_1) + \varrho_{q,x_0,R,\mu_{\max},w_{\min},\alpha}(x,y,t_1,t_2))$$

as was claimed.

q.e.d.

6. Examples

In this section we show that our curvature notion behaves somewhat as expected, by computing curvature lower bounds for certain classes of graphs. We also show that $\mathbb{Z}^d$ admits strong cut-off functions in the sense of Definition 4.24.

6.1. General graphs and trees. Here we prove that every graph satisfies $CDE\left(2, -D_\mu\left(\frac{D_w}{2}+1\right)\right)$. We show that this bound is close to sharp for graphs that are locally trees; in particular the curvature of a D-regular large girth graph goes to $-\infty$ linearly as $D \to \infty$.

Theorem 6.1. *Suppose G is any graph with $D_w = \max_{x\sim y} \frac{\deg(x)}{w_{xy}}$ and $D_\mu = \max \frac{\deg(x)}{\mu(x)}$. Then G satisfies $CDE\left(2, -D_\mu\left(\frac{D_w}{2}+1\right)\right)$.*

Proof. Fix a function $f : V \to \mathbb{R}$ with $f > 0$, and vertex x so that $\Delta f(x) < 0$. We begin by calculating:

$$\begin{aligned}
\widetilde{\Gamma}_2(f)(x) =& \frac{1}{2}\left[\Delta\Gamma(f) - 2\Gamma\left(f, \frac{\Delta f^2}{2f}\right)\right] \\
=& \frac{1}{2}\left[\widetilde{\sum_{y\sim x}}(\Gamma(f)(y) - \Gamma(f)(x))\right. \\
&\left. - \frac{1}{2}\widetilde{\sum_{y\sim x}}(f(y)-f(x))\left(\frac{(\Delta f^2)(y)}{f(y)} - \frac{(\Delta f^2)(x)}{f(x)}\right)\right] \\
=& \frac{1}{4}\widetilde{\sum_{y\sim x}\sum_{z\sim y}}\left[(f(z)-f(y))^2 - (f(y)-f(x))\frac{(f^2(z)-f^2(y))}{f(y)}\right] \\
&- \frac{1}{2}\widetilde{\sum_{y\sim x}}\Gamma(f)(x) + \frac{1}{4}\widetilde{\sum_{y\sim x}}(f(y)-f(x))\frac{(\Delta f^2)(x)}{f(x)} \\
=& \frac{1}{4}\widetilde{\sum_{y\sim x}\sum_{z\sim y}}\left[\frac{f(x)}{f(y)}f^2(z) - 2f(y)f(z) + 2f^2(y) - f(x)f(y)\right] \\
&- \frac{1}{2}\widetilde{\sum_{y\sim x}}\Gamma(f)(x) + \frac{1}{2}\left((\Delta f(x))^2 + \frac{\Gamma(f)}{f(x)}(\Delta f)\right), \qquad (6.2)
\end{aligned}$$

where in the second to last line we collected the terms at distance two, and in the last line we used the identity that $(\Delta f^2)(x) = 2f(x)(\Delta f)(x) + 2\Gamma(f)(x)$.

The summands of the double sum are quadratics in $f(z)$. They are minimized when $f(z) = \frac{f^2(y)}{f(x)}$, whence the summand is $-\frac{f(y)}{f(x)}(f(x) - f(y))^2$, so

$$\begin{aligned}
\widetilde{\Gamma}_2(f) \geq& -\frac{1}{4}\widetilde{\sum_{y\sim x}\sum_{z\sim y}}\frac{f(y)}{f(x)}(f(x)-f(y))^2 \qquad (6.3) \\
&- \frac{1}{2}\widetilde{\sum_{y\sim x}}\Gamma(f)(x) + \frac{1}{2}\left((\Delta f(x))^2 + \frac{\Gamma(f)}{f(x)}(\Delta f)\right) \\
\geq& -\frac{1}{4}D_\mu\widetilde{\sum_{y\sim x}}\frac{f(y)}{f(x)}(f(x)-f(y))^2 \\
&- \frac{1}{2}D_\mu\Gamma(f)(x) + \frac{1}{2}\left((\Delta f(x))^2 + \frac{\Gamma(f)}{f(x)}(\Delta f)\right).
\end{aligned}$$

We use the fact that

$$\Delta f = \widetilde{\sum_{y\sim x}}(f(y) - f(x)) \geq -\widetilde{\sum_{y\sim x}} f(x) \geq -D_\mu f(x)$$

to lower bound the $\frac{\Gamma(f)}{f(x)}(\Delta f)$ term. Finally, we use the fact that $\Delta f < 0$, and Lemma 4.3 (i) implies that

$$\frac{f(y)}{f(x)} < D_w.$$

Therefore, continuing from (6.3),

$$\begin{aligned}\widetilde{\Gamma}_2(f) &\geq -\frac{1}{4} D_\mu \widetilde{\sum_{y\sim x}} \frac{f(y)}{f(x)}(f(x) - f(y))^2 - \frac{1}{2} D_\mu \Gamma(f)(x) \\ &+ \frac{1}{2}\left((\Delta f(x))^2 + \frac{\Gamma(f)}{f(x)}(\Delta f)\right) > \frac{1}{2}(\Delta f(x))^2 - D_\mu\left(\frac{D_w}{2} + 1\right)\Gamma(f)\end{aligned}$$

as desired.

q.e.d.

6.2. Sharpness of Theorem 6.1 on trees. For unweighted graphs with the normalized Laplacian, Theorem 6.1 states that all graphs satisfy $CDE(2, -\frac{D}{2} - 1)$. Such a lower bound on curvature is essentially tight in the case of trees. Indeed, let (T_D, x_0) denote the infinite D-ary tree rooted at x_0. We find below functions f_D for which

$$\frac{\widetilde{\Gamma}_2(f_D)}{\Gamma(f_D)} \leq -(1 + o(1))\frac{D}{2}, \text{ as } D \to \infty. \tag{6.4}$$

To construct the function f_D we do the following. Let $y_1, \ldots, y_D$ denote the neighbors of x_0. We define functions f_ϵ as follows:

$$\begin{aligned} f_\epsilon(x_0) &= 1 \\ f_\epsilon(y_1) &= (1-\epsilon)D \\ f_\epsilon(y_i) &= \epsilon \qquad\qquad \text{for } 2 \leq i \leq D. \end{aligned}$$

For vertices $z \sim y_i$ at distance two from x_0, we take $f_\epsilon(z) = f^2(y_i)$ (and hence by the computation in the proof of Theorem 6.1 being the value that minimizes $\widetilde{\Gamma}_2(f_\epsilon)$ given the $f_\epsilon(y_i)$). Then we take $f_D = f_\epsilon$ for $\epsilon = D^{-3/2}$. It is a straightforward computation to verify that (6.4) holds.

6.3. Ricci-flat graphs. Chung and Yau [**7**] introduced the notion of Ricci-flat (unweighted) graphs as a generalization of abelian Cayley graphs.

Definition 6.5. A d-regular graph $G(V, E)$ is Ricci-flat at the vertex $x \in V$ if there exist maps $\eta_i : V \to V$; $i = 1, \ldots, d$ that satisfy the following conditions.

1) $x\eta_i(x) \in E$ for every $i = 1, \ldots, d$.
2) $\eta_i(x) \neq \eta_j(x)$ for every $i \neq j$.
3) For every i we have $\cup_j \eta_i(\eta_j(x)) = \cup_j \eta_j(\eta_i(x))$.

In fact, to test Ricci-flatness at x it is sufficient for the η_is to be defined only on x and the vertices adjacent to x.

Finally, the graph G is Ricci-flat if it is Ricci-flat at every vertex.

Given a weighted graph which is Ricci-flat when viewed as an unweighted graph, the weighting is called *consistent* if

1) There exist numbers $w_1, \ldots, w_d$ so that $w_{x\eta_i(x)} = w_i$ for all $i = 1, \ldots, d$ and $x \in V$.
2) Whenever $\eta_j(\eta_i(x)) = \eta_i(\eta_k(x))$ for some $x \in V$, then $w_j = w_k$.
3) The weights are symmetric, so $w_{xy} = w_{yx}$ whenever $x \sim y$.

If only the first two conditions hold (so the weights are not necessarily symmetric) then we say the weighting is *weakly consistent.*

Remark 6.6. The conditions on the weights are fairly restrictive, but there are two cases when they are easily seen to be satisfied.

1) If $w_i = 1 : i = 1, \ldots, d$ then we get back the original notion of a Ricci-flat graph.
2) If G is Ricci-flat, and the functions η_i locally commute, that is $\eta_i(\eta_j(x)) = \eta_j(\eta_i(x))$, then any sequence $w_1, \ldots, w_d$ can be used to introduce a weakly consistent weighting for G.

The critical reason why we choose these restrictions is the following: If G is a (weakly) consistently weighted Ricci-flat graph and $f : V \to \mathbb{R}$ is a function, then for any vertex $x \in V$, and $1 \leq i \leq d$,

$$\sum_j w_j f(\eta_i \eta_j(x)) = \sum_j w_j f(\eta_j \eta_i(x)). \tag{6.7}$$

Here the fact G is Ricci flat implies the sums are over the same set of vertices, and the second condition on the weights ensures that the sums are equal.

Theorem 6.8. *Let G be a d-regular Ricci-flat graph. Suppose that the measure μ defining Δ satisfies $\mu(x) \equiv \mu$ for all vertices $x \in G$.*

1) *If the weighting of G is consistent, then G satisfies $CDE(d, 0)$.*
2) *If the weighting of G is weakly consistent, then G satisfies $CDE(\infty, 0)$*

Remark 6.9. For a d-regular Ricci-flat graph and a weakly consistent weighting, the two standard choices of the measure $\mu \equiv 1$ and $\mu(x) = \deg(x)$ satisfy $\mu(x) \equiv \mu$ for all $x \in V$.

Corollary 6.10. The usual Cayley graph of $\mathbb{Z}^k$ satisfies $CDE(2k, 0)$, for the regular or normalized graph Laplacian.

Proof of Theorem 6.8. Let $f : V \to \mathbb{R}$ be a function.

We begin by assuming that G is Ricci-flat, and the weighting is weakly consistent.

We will write y for $f(x)$, y_i for $f(\eta_i(x))$, and y_{ij} for $f(\eta_j(\eta_i(x)))$. With this notation we have

$$\begin{aligned}\Delta\Gamma(f)(x) &= \frac{1}{\mu}\sum_i w_i\left(\Gamma(f)(\eta_i(x)) - \Gamma(f)(x)\right)\\ &= \frac{1}{2\mu^2}\sum_i\sum_j w_iw_j\left((y_{ij}-y_i)^2 - (y_j-y)^2\right)\\ &= \frac{1}{2\mu^2}\sum_{i,j} w_iw_j((y_{ij}^2 - y_j^2) + (y_i^2 - y^2) - 2y_iy_{ij} + 2yy_j),\end{aligned}$$

and

$$\begin{aligned}&2\Gamma\left(f, \frac{\Delta f^2}{2f}\right) =\\ &= \frac{1}{2\mu^2}\sum_i\sum_j w_iw_j(y_i - y)\left(\frac{y_{ij}^2 - y_i^2}{y_i} - \frac{y_j^2 - y^2}{y}\right)\\ &= \frac{1}{2\mu^2}\sum_i\sum_j w_iw_j(y_i - y)\left(\frac{y_{ji}^2 - y_i^2}{y_i} - \frac{y_j^2 - y^2}{y}\right)\\ &= \frac{1}{2\mu^2}\sum_i\sum_j w_iw_j(y_j - y)\left(\frac{y_{ij}^2 - y_j^2}{y_j} - \frac{y_i^2 - y^2}{y}\right)\\ &= \frac{1}{2\mu^2}\sum_i\sum_j w_iw_j\left((y_{ij}^2 - y_j^2) + (y_i^2 - y^2) + 2yy_j - \frac{y^2y_{ij}^2 + y_i^2y_j^2}{yy_j}\right).\end{aligned}$$

Here, the second equality follows from the (weakly) consistent labeling as observed in (6.7) and the third equality follows from changing the role of i and j.

Combining, we see

$$\begin{aligned}\widetilde{\Gamma}_2(f) &= \frac{1}{2}\left(\Delta\Gamma(x) - 2\Gamma\left(f, \frac{\Delta f^2}{2f}\right)\right)\\ &= \frac{1}{4\mu^2}\sum_{ij} w_iw_j\left(\frac{y^2y_{ij}^2 - 2y_iy_jy_{ij}y + y_i^2y_j^2}{yy_j}\right)\\ &= \frac{1}{4\mu^2}\sum_{ij} w_iw_j\frac{(yy_{ij} - y_iy_j)^2}{yy_j}. \qquad (6.11)\end{aligned}$$

Clearly, $\widetilde{\Gamma}_2(f) \geq 0$, so G satisfies $CDE(\infty, 0)$, proving the first part of the assertion.

Now we further assume that the weighting of G is consistent. (That is, we further assume the weights are symmetric.) Now for each i there is a unique $j = j(i)$ such that $\eta_j(\eta_i(x)) = x$ and thus $y_{ij} = y$. Throwing away all the other terms from (6.11) we get:

$$\widetilde{\Gamma}_2 \geq \frac{1}{4\mu^2} \sum_i w_i w_{j(i)} \frac{(y^2 - y_i y_{j(i)})^2}{y y_i}.$$

Note that $j(i)$ is a full permutation, and the symmetry of weights implies that $w_i = w_{j(i)}$, and hence on the cycles in $j(i)$ the weights are constant. Suppose the permutation $j(i)$ decomposes into cycles $C_1, \dots, C_k$, with lengths $\ell_1, \dots, \ell_k$. We focus our attention on an arbitrary cycle C. Then there exists a w_C, and the terms above corresponding to this cycle are of the form

$$\begin{aligned}\frac{w_C^2}{4\mu^2} \sum_{i \in C} \frac{(y^2 - y_i y_{j(i)})^2}{y y_i} &= \frac{w_C^2 y^2}{4\mu^2} \sum_{i \in C} \frac{(1 - z_i z_{j(i)})^2}{z_i} \\ &= \frac{w_C^2 y^2}{4\mu^2} \sum_{i \in C} \left(\frac{1}{z_i} - 2 z_{j(i)} + z_i z_{j(i)}^2 \right),\end{aligned}$$

where we take $z_i = y_i / y$. We can assume without loss of generality that $j(i)$ restricted to this cycle C is a permutation on $[\ell]$, and $0 < z_1 \leq z_2 \leq \cdots \leq z_\ell$. We can apply the Rearrangement Inequality to obtain $\sum z_i z_{j(i)}^2 \geq \sum z_i z_{\ell+1-i}^2$ and hence

$$\begin{aligned}&\frac{w_C^2 y^2}{4\mu^2} \sum_{i \in C} \left(\frac{1}{z_i} - 2 z_{\ell+1-i} + z_i z_{\ell+1-i}^2 \right) \\ &\qquad = \frac{w_C^2 y^2}{8\mu^2} \sum_{i \in C} (1 - z_i z_{\ell+1-i})^2 \left(\frac{1}{z_i} + \frac{1}{z_{\ell+1-i}} \right) \\ &\qquad \geq \frac{w_C^2 y^2}{4\mu^2} \sum_{i \in C} \frac{(1 - z_i z_{\ell+1-i})^2}{\sqrt{z_i z_{\ell+1-i}}} \\ &\qquad \geq \frac{w_C^2 y^2}{\mu^2} \sum_{i \in C} (1 - \sqrt{z_i z_{\ell+1-i}})^2 \\ &\qquad = \frac{1}{\mu^2} \sum_{i \in C} (w_C (y - \sqrt{y_i y_{\ell+1-i}}))^2. \qquad (6.12)\end{aligned}$$

We now combine the cycles together and apply Cauchy-Schwarz, to see

$$\widetilde{\Gamma}_2(f) \geq \frac{1}{d} \left(\frac{1}{\mu} \sum_i w_i (y - \sqrt{y_i y_{i'}}) \right)^2, \qquad (6.13)$$

where $y_{i'}$ is the partner of y_i in its cycle as given in (6.12).

Finally, we assume that $\Delta f(x) < 0$ to prove CDE conditions. This implies that $\sum_i w_i y_i < \sum_i w_i y$. Also from the fact that y_i and y'_i appear in the same cycle, we have $\sum_i w_i y'_i = \sum_i w_i y_i$. Applying Cauchy-Schwarz we see that

$$\sum_i w_i \sqrt{y_i y_{i'}} \leq \sqrt{\left(\sum_i w_i y_i\right)\left(\sum_i w_i y'_i\right)} = \sum_i w_i y_i < \sum_i w_i y.$$

Thus continuing (6.13), we see the interior square is positive, and hence

$$\begin{aligned}\widetilde{\Gamma}_2(f) &\geq \frac{1}{d}\left(\frac{1}{\mu}\sum_i w_i(y - \sqrt{y_i y_{i'}})\right)^2 \\ &\geq \frac{1}{d}\left(\frac{1}{\mu}\sum_i w_i(y - y_i)\right)^2 = \frac{1}{d}(\Delta f)^2\end{aligned}$$

as desired. q.e.d.

6.4. Strong cut-off function in $\mathbb{Z}^d$.

Proposition 6.14. *The usual Cayley graph of* $\mathbb{Z}^d$*, along with a strongly consistent weighting, admits a* $(100, R)$*-strong cut-off function supported in a ball of radius* $\sqrt{d}R$ *centered at the origin.*

Remark 6.15. In the case of the Cayley graph of $\mathbb{Z}^d$, a strongly consistent weighting just means that for each of the d generators e_i, $w_{xe_i(x)} = w_{xe_i^{-1}(x)}$.

We did not attempt to optimize the constant 100 appearing in this statement.

Proof. For a vertex $x \in \mathbb{Z}^d$ let $x_i \in \mathbb{Z}$ denote its ith coordinate and write $|x|^2 = \sum_i x_i^2$. We are going to prove that the function

$$\phi(x) = \left(\max\left\{0, \frac{R^2 - |x|^2}{R^2}\right\}\right)^2$$

is a $(100, R)$-strong cut-off function centered at the origin. It is supported in a "Euclidean" ball of radius R which is contained in a ball of radius $\sqrt{d}R$ measured in the graph distance.

We need to show that one of the two cases in Definition 4.24 is satisfied. If $R^2 - |x|^2 \leq 10R$ then the first case is clearly satisfied, so we may assume $R^2 - |x|^2 > 10R$. Also, $|x_i| < R$ for any i; otherwise $\phi(x)$ would be 0. These together imply that

$$\frac{R^2 - |x|^2}{R^2 - |x|^2 \pm 2|x_i| + 1} \leq \frac{1}{1 - \frac{2|x_i| - 1}{R^2 - |x|^2}} \leq \frac{1}{1 - \frac{3R}{10R}} \leq \frac{10}{7}. \tag{6.16}$$

By the consistency, for each coordinate there is a single weight w_i. Now we can compute

$$\begin{aligned}
&\mu(x)\phi^2(x)\Delta\frac{1}{\phi}(x)\\
&\qquad= \left(\frac{R^2-|x|^2}{R^2}\right)^4\frac{R^4}{2}\cdot\sum_i w_i\left(\frac{1}{(R^2-|x|^2-2|x_i|-1)^2}\right.\\
&\qquad\qquad\left.+\frac{1}{(R^2-|x|^2+2|x_i|-1)^2}-\frac{2}{(R^2-|x|^2)^2}\right)\\
&\qquad\qquad\qquad= \left(\frac{R^2-|x|^2}{R^2}\right)^2\cdot\sum_i w_i\cdot\\
&\cdot\left(\frac{(R^2-|x|^2)^2((R^2-|x|^2-1)^2+4x_i^2)-((R^2-|x|^2-1)^2-4x_i^2)^2}{(R^2-|x|^2-2|x_i|-1)^2(R^2-|x|^2+2|x_i|-1)^2}\right)\\
&\quad\leq\frac{1}{R^4}\sum_i w_i\left(\frac{12x_i^2(R^2-|x|^2)^4+2(R^2-|x|^2)^5}{(R^2-|x|^2-2|x_i|-1)^2(R^2-|x|^2+2|x_i|-1)^2}\right).
\end{aligned}$$

In the last line, we used that $(R^2-|x|^2-1)\leq(R^2-|x|^2)$ and discarded some negative terms. Then using (6.16) along with $x_i^2<R^2$ and $R^2-|x|^2<R^2$, we have

$$\phi^2(x)\Delta\frac{1}{\phi}(x)\leq\frac{1}{\mu(x)}\sum_i w_i\left(2\cdot\frac{(10/7)^4}{R^2}\right)<\frac{100}{R^2}D_\mu.$$

A computation similar in spirit, but less complicated, shows that

$$\begin{aligned}
&\phi^3(x)\Gamma\left(\frac{1}{\phi}\right)(x)=\frac{(R^2-|x|^2)^6}{2R^{12}\mu(x)}\\
&\qquad\cdot\sum_i w_i\left|\frac{R^4}{(R^2-|x|^2)^2}-\frac{R^4}{(R^2-|x|^2\pm2|x_i|-1)^2}\right|^2\leq\frac{100}{R^2}D_\mu,
\end{aligned}$$

and thus ϕ indeed is a $(100,R)$-strong cut-off function. q.e.d.

7. Applications

7.1. Heat kernel estimates and volume growth. One of the fundamental applications of the Li-Yau inequality, and more generally parabolic Harnack inequalities, is the derivation of heat kernel estimates. As alluded to in the introduction, Grigor'yan and Saloff-Coste (in the manifold setting) and Delmotte (in the graph setting) proved the equivalence of several conditions (including Harnack inequalities, and the combination of volume doubling and the Poincaré inequality) to the heat kernel satisfying the following Gaussian-type bounds. Let $P_t(x,y)$ denote the fundamental solution to the heat equation starting at x.

Definition 7.1. G satisfies the Gaussian heat-kernel property $\mathcal{G}(c, C)$ if $d(x, y) \leq t$ implies

$$\frac{c}{\operatorname{vol}(B(x, \sqrt{t}))} \exp\left(-C\frac{d(x,y)^2}{t}\right) \leq P_t(x, y) \leq \frac{C}{\operatorname{vol}(B(x, \sqrt{t}))} \exp\left(-c\frac{d(x,y)^2}{t}\right).$$

In the graph setting, Delmotte proved that $\mathcal{G}(c, C)$ is equivalent to two other (sets of) properties. The first is the pair of volume doubling and Poincaré.

Definition 7.2. G satisfies the volume doubling property $\mathcal{VD}(C)$ if for all $x \in V$ and all $r \in \mathbb{R}^+$:

$$\operatorname{vol}(B(x, 2r)) \leq C\operatorname{vol}(B(x, r)).$$

Definition 7.3. G satisfies the Poincaré inequality $\mathcal{P}(C)$ if

$$\sum_{x\in B(x_0,r)} \mu(x)(f(x) - f_B)^2 \leq Cr^2 \sum_{x,y\in B(x_0,2r)} w_{xy}(f(y) - f(x))^2,$$

for all $f : V \to \mathbb{R}$, for all $x_0 \in V$, and for all $r \in \mathbb{R}^+$, where

$$f_B = \frac{1}{\operatorname{vol}(B(x_0, r))} \sum_{x\in B(x_0,r)} \mu(x)f(x).$$

The final equivalent condition is a Harnack inequality in the following form:

Definition 7.4. Fix $0 < \theta_1 < \theta_2 < \theta_3 < \theta_4$ and $C > 0$. G satisfies the Harnack inequality property $\mathcal{H}(\theta_1, \theta_2, \theta_3, \theta_4, C)$ if for all $x_0 \in V$ and $s, R \in \mathbb{R}^+$, and every positive solution $u(x, t)$ to the heat equation on $Q = B(x_0, 2R) \times [s, s + \theta_4 R^2]$,

$$\sup_{Q^-} u(x, t) \leq C \inf_{Q^+} u(x, t),$$

where $Q^- = B(x_0, R) \times [s + \theta_1 R^2, s + \theta_2 R^2]$, and $Q^+ = B(x_0, R) \times [s + \theta_3 R^2, s + \theta_4 R^2]$.

Delmotte shows that $\mathcal{H}(\theta_1, \theta_2, \theta_3, \theta_4, C_0) \Leftrightarrow \mathcal{P}(C_1) + \mathcal{VD}(C_2) \Leftrightarrow \mathcal{G}(c_3, C_4)$ for graphs; the equivalent statement for manifolds is due to Grigor'yan and Saloff-Coste. In the manifold case, it is well known that non-negative curvature implies $\mathcal{VD}$ and $\mathcal{P}$, but on graphs it is not known. Here, we show that $CDE(n, 0)$ implies $\mathcal{H}$ (and hence all the properties) under the assumption that G admits a $(c, \eta R)$, strong cut-off function contained in a ball $B(x_0, R)$ around every point. For instance, the strong cut-off function for the integer lattice $\mathbb{Z}^d$ shows we can guarantee a $(c, \frac{1}{\sqrt{d}}R)$, strong cut-off function in balls of radius R.

Corollary 7.5 (Corollary of Theorem 5.2)**.** Suppose G satisfies $CDE(n,0)$, and let $\eta \in (0,1)$. If for every $x \in B(x_0,R)$ G admits a $(c,\eta R)$-strong cut-off function centered at x with support in $B(x_0,2R)$ then G satisfies $\mathcal{H}(\theta_1,\theta_2,\theta_3,\theta_4,C_0)$ for some C_0 (and therefore $\mathcal{G}(c,C)$, $\mathcal{P}(C)$, and $\mathcal{VD}(C)$ for appropriate constants).

Proof. The proof is almost immediate from Theorem 5.2. Fix $\theta_1 < \theta_2 < \theta_3 < \theta_4$. From Theorem 4.26 G satisfies a gradient estimate of the form

$$2(1-\alpha)\frac{\Gamma(\sqrt{u})}{u} - \frac{\Delta u}{u} \leq \frac{c_1}{t} + \frac{c_2}{R^2}$$

on $B(x_0,R)$. For $T_1 \in [s+\theta_1 R^2, s+\theta_2 R^2]$ and $T_2 \in [s+\theta_3 R^2, s+\theta_4 R^2]$,

$$\frac{T_2}{T_1} \leq \frac{s+\theta_4 R^2}{s+\theta_1 R^2} \leq 1 + \frac{(\theta_4-\theta_1)R^2}{s+\theta_4 R^2} \leq 1 + \frac{\theta_4-\theta_1}{\theta_4}.$$

Furthermore

$$\frac{c_2}{R^2}\cdot(T_2-T_1) \leq c_2(\theta_4-\theta_1)$$

and

$$\frac{d(x,y)^2}{T_2-T_1} \leq \frac{4}{\theta_3-\theta_2}.$$

Thus each of the terms arising in the Harnack inequality derived in Theorem 5.2 are bounded by constants not depending on s, x_0, and R, so we can choose a C_0 guaranteeing that $\mathcal{H}(\theta_1,\theta_2,\theta_3,\theta_4,C_0)$ holds.

q.e.d.

In general, however, we only have for graphs satisfying $CDE(n,0)$ the gradient estimate derived from Theorem 4.20. Using this gradient estimate in Theorem 5.2 implies that

$$u(x,T_1) \leq u(y,T_2)\cdot\left(\frac{T_2}{T_1}\right)^{c_1} \exp\left(\frac{c_2}{R}(T_2-T_1) + c_3\frac{d(x,y)^2}{T_2-T_1}\right).$$

This will not suffice for proving $\mathcal{H}(\theta_1,\theta_2,\theta_3,\theta_4,C_0)$. Indeed, if $T_2 - T_1 = cR^2$, then this only implies that

$$\sup_{Q^-} u(x,t) \leq \exp(cR + c')\inf_{Q^+} u(x,t),$$

where the constant depends now on R.

Nevertheless, we can derive heat kernel upper bounds that are Gaussian, and lower bounds that are not quite Gaussian but still have a similar form. The heat kernel bound then allows us to derive volume growth bounds: we show that if G satisfies $CDE(n,0)$ then G has polynomial volume growth. We derive here only on-diagonal upper and lower bounds, but it is known that off-diagonal bounds can be established using the on-diagonal bounds.

Theorem 7.6. *Suppose G satisfies $CDE(n,0)$ and has maximum degree D. Then there exist constants so that, for $t>1$,*

$$C\frac{1}{t^n}\exp\left(-C'\frac{d^2(x,y)}{t-1}\right) \le P_t(x,y) \le C''\frac{\mu(y)}{\mathrm{vol}(B(x,\sqrt{t}))}.$$

Proof. The upper bound is standard and follows from the methods of Delmotte from [**10**]. Indeed, observe that the only time a Harnack inequality is utilized in the proof of the upper bound, it is used on a solution to the heat equation which is not just in the ball, but everywhere. For such a function, letting $R\to\infty$ we observe that if u is a solution on the whole graph, with $c_1=n$, then

$$u(x,T_1) \le u(y,T_2)\left(\frac{T_2}{T_1}\right)^n \exp\left(\frac{4d(x,y)^2D}{(1-\alpha)(T_2-T_1)}\right). \tag{7.7}$$

Then the argument proceeds as follows. Let $P_\cdot(\cdot,y)$ be the fundamental solution to the heat equation. Then by (7.7), for $u=P_t$ if $z\in B(x,\sqrt{t})$,

$$P_t(x,y) \le P_{2t}(z,y)2^n\exp\left(\frac{D}{1-\alpha}\right) = C'\cdot P_{2t}(z,y).$$

Thus

$$\begin{aligned}P_t(x,y) &\le \frac{C}{\mathrm{vol}(B(x,\sqrt{t}))}\sum_{z\in B(x,\sqrt{t})}\mu(z)P_{2t}(z,y)\\ &\le \frac{C}{\mathrm{vol}(B(x,\sqrt{t}))}\sum_{z\in B(x,\sqrt{t})}\mu(y)P_{2t}(y,z)\\ &\le \frac{C'\mu(y)}{\mathrm{vol}(B(x,\sqrt{t}))}.\end{aligned}$$

This gives the desired upper bound.

The lower bound proceeds directly from the Harnack inequality (7.7). Indeed,

$$P_1(y,y) \le P_t(x,y)t^n\exp\left(C'd(x,y)^2/(t-1)\right).$$

Noting that $P_1(y,y)$ is bounded from below by an absolute constant in a bounded degree graph, and dividing, yield the result. q.e.d.

An immediate corollary of Theorem 7.6 is polynomial volume growth.

Corollary 7.8. Let G be a graph satisfying $CDE(n,0)$. Then G has a polynomial volume growth.

Proof. Applying Theorem 7.6 with $y=x$ gives

$$\frac{C}{t^n} \le \frac{C'\mu(x)}{\mathrm{vol}(B(x,\sqrt{t}))},$$

and cross multiplying yields the desired bounds. q.e.d.

7.2. Buser's inequality for graphs. As another application of the gradient estimate in Theorem 4.10 we prove a Buser-type [**6**] estimate for the smallest nontrivial eigenvalue of a finite graph. From now on we assume that the edge weights are symmetric, i.e. $w_{xy} = w_{yx}$ for all $x \sim y$.

In the following we denote

$$\|f\|_p = \left(\sum_{x\in V} \mu(x) f^p(x)\right)^{\frac{1}{p}} \text{ and } \|f\|_\infty = \sup_{x\in V} |f(x)|.$$

The Cheeger constant h of a graph is defined as

$$h = \inf_{\emptyset \neq U\subset V:\mathrm{vol}(U)\leq 1/2\,\mathrm{vol}(V)} \frac{|\partial U|}{\mathrm{vol}(U)},$$

where $|\partial U| = \sum_{x\in U, y\in V\setminus U} w_{xy}$ and $\mathrm{vol}(U) = \sum_{x\in U} \mu(x)$.

Theorem 7.9. *Let G be a finite graph satisfying $CDE(n, -K)$ for some $K > 0$ and fix $0 < \alpha < 1$. Then*

$$\lambda_1 \leq \max\{2C\sqrt{K}h, 4C^2h^2\},$$

where the constant

$$C = 8\left(3\mu_{\max}\frac{(2-\alpha)n}{\alpha(1-\alpha)^2 w_{\min}}\right)^{\frac{1}{2}}$$

only depends on the dimension n and $\mu_{\max}$.

Remark 7.10.

- By using Theorem 4.4 instead of Theorem 4.10, one obtains the same statement in the case of $K = 0$ where now the constant C is given by $C = 8\sqrt{3n\mu_{\max}}$.
- The Cheeger inequality states that $\frac{h^2}{2D_\mu} \leq \lambda_1$. Thus in particular if $K = 0$, Theorem 7.9 implies that $\frac{h^2}{2D_\mu} \leq \lambda_1 \leq 4C^2h^2$, i.e. λ_1 is of the order h^2.
- Klartag and Kozma [**16**] show a similar but stronger result for graphs satisfying the original CD-inequality. Namely, they prove, following the arguments of Ledoux [**18**], that if a finite graph satisfies $CD(\infty, -K)$ then

  $$\lambda_1 \leq 8\max\{\sqrt{K}h, h^2\}.$$

  Note that their condition does not involve dimension, and hence their constant is also dimension independent.

We divide the proof into several different steps, closely following Ledoux's [**17**] argument on compact manifolds. The proof of the following lemma is based on ideas by Varopoulos [**29**].

Lemma 7.11. *Let G be a finite graph satisfying $CDE(n,-K)$ for some $K>0$, and let P_tf be a positive solution to the heat equation on G. Fix $0<\alpha<1$ and let $0<t\le t_0$; then*

$$\|\Gamma(P_tf)\|_\infty \le \frac{12c}{(1-\alpha)t}\|f\|_\infty^2,$$

where $c=\frac{n}{2(1-\alpha)}+\frac{Kn}{\alpha}t_0$.

Proof. On the one hand, by the gradient estimate in Theorem 4.10 and $t\le t_0$,

$$\frac{(1-\alpha)\Gamma(\sqrt{P_tf})}{P_tf}-\frac{\Delta P_tf}{2P_tf}\le \frac{n}{2(1-\alpha)t}+\frac{Kn}{\alpha}\frac{t_0}{t}=:\frac{c}{t}.$$

Since $\frac{(1-\alpha)\Gamma(\sqrt{P_tf})}{P_tf}\ge 0$, and the estimate is trivial if $\frac{\Delta P_tf}{2P_tf}\ge 0$, we conclude that

$$\left(\frac{\Delta P_tf}{2P_tf}\right)^-\le\frac{c}{t}, \tag{7.12}$$

where $(\quad)^\pm$ denotes the positive and negative part, respectively. Note that $0=\sum_{x\in V}\mu(x)\Delta P_tf(x)=\sum_{x\in V}\mu(x)(\Delta P_tf)^+(x)-\mu(x)(\Delta P_tf)^-(x)$ which implies

$$\begin{aligned}\sum_{x\in V}\mu(x)\left(\Delta P_tf\right)^-(x) \\ =\frac{1}{2}\sum_{x\in V}\mu(x)((\Delta P_tf)^-(x)+(\Delta P_tf)^+(x))=\frac{1}{2}\|\Delta P_tf\|_1.\end{aligned} \tag{7.13}$$

Moreover, since $\sum_{x\in V}\mu(x)P_tf(x)=\sum_{x\in V}\mu(x)f(x)$ and $f>0$ it follows from (7.12) and (7.13) that

$$\frac{1}{4}\|\Delta P_tf\|_1=\frac{1}{2}\sum_{x\in V}\mu(x)\left(\Delta P_tf\right)^-\le\frac{c}{t}\sum_{x\in V}\mu(x)P_tf(x)=\frac{c}{t}\|f\|_1. \tag{7.14}$$

It is well known that for bounded linear operators $T:\ell^p\to\ell^q$ and their dual operators $T^*:\ell^{q^*}\to\ell^{p^*}$ it holds that

$$\|T\|_{\ell^p\to\ell^q}=\|T^*\|_{\ell^{q^*}\to\ell^{p^*}}$$

where

$$\|T\|_{A\to B}:=\sup_{f\in A}\frac{\|Tf\|_B}{\|f\|_A}$$

and p and p^* are Hölder conjugate exponents, i.e. $\frac{1}{p}+\frac{1}{p^*}=1$. Since ΔP_t is self-adjoint we have for all f

$$\frac{\|\Delta P_tf\|_\infty}{\|f\|_\infty}\le\|\Delta P_t\|_{\infty\to\infty}=\|\Delta P_t\|_{1\to1}=\sup_{g\in\ell^1}\frac{\|\Delta P_tg\|_1}{\|g\|_1}\le\frac{4c}{t}.$$

On the other hand, it follows from the gradient estimate by applying the infinity norm on both sides that

$$\begin{aligned}(1-\alpha)\|\Gamma(\sqrt{P_t f})\|_\infty &\leq \frac{1}{2}\|\Delta P_t f\|_\infty + \frac{c}{t}\|P_t f\|_\infty \\ &\leq \frac{2c}{t}\|f\|_\infty + \frac{c}{t}\|f\|_\infty = \frac{3c}{t}\|f\|_\infty \end{aligned} \tag{7.15}$$

where we used (7.14) and $\|P_t f\|_\infty \leq \|P_0 f\|_\infty = \|f\|_\infty$ for all $t > 0$. Now the proof is almost complete; we only need to estimate $\Gamma(\sqrt{P_t f})$ by $\Gamma(P_t f)$. It is easy to see that $\Gamma(u) \leq 4\|u\|_\infty \Gamma(\sqrt{u})$ for all positive functions $u > 0$. Indeed,

$$\begin{aligned}\Gamma(u)(x) &= \frac{1}{2\mu(x)}\sum_{y\sim x} w_{xy}\,(u(x)-u(y))^2 \\ &= \frac{1}{2\mu(x)}\sum_{y\sim x} w_{xy}\left(\sqrt{u(x)}-\sqrt{u(y)}\right)^2\left(\sqrt{u(x)}+\sqrt{u(y)}\right)^2 \\ &\leq 4\|u\|_\infty\Gamma(\sqrt{u}).\end{aligned}$$

Using this in (7.15) we obtain

$$\|\Gamma(P_t f)\|_\infty \leq \frac{12c}{(1-\alpha)t}\|f\|_\infty^2,$$

which finishes the proof. q.e.d.

Remark 7.16. Using the notation $|\nabla f| = \sqrt{\Gamma(f)}$, the statement of the last lemma is equivalent to

$$\||\nabla P_t f|\|_\infty \leq 2\sqrt{\frac{3c}{(1-\alpha)t}}\|f\|_\infty. \tag{7.17}$$

Lemma 7.18. *Let G be a finite graph satisfying $CDE(n,-K)$ for some $K > 0$, and let $P_t f$ be a positive solution to the heat equation on G. Fix $0 < \alpha < 1$ and let $0 < t \leq t_0$ then*

$$\|f - P_t f\|_1 \leq 8\sqrt{\frac{3c}{1-\alpha}}\||\nabla f|\|_1\sqrt{t},$$

where c is the constant in Lemma 7.11.

Proof. For any positive function g we have

$$\begin{aligned}&\sum_{x\in V}\mu(x)g(x)(f-P_t f)(x) = \sum_{x\in V}\mu(x)g(x)(P_0 f - P_t f)(x) \\ &= -\int_0^t \sum_{x\in V}\mu(x)g(x)\frac{\partial}{\partial s}P_s f(x)ds = -\int_0^t\sum_{x\in V}\mu(x)g(x)\Delta P_s f(x)ds \\ &\quad = -\int_0^t\sum_{x\in V}\mu(x)P_s g(x)\Delta f(x)ds = \int_0^t\sum_{x\in V}\mu(x)\Gamma(P_s g, f)(x)ds,\end{aligned}$$

where we used that $P_s = e^{s\Delta}$ is self-adjoint, P_s commutes with Δ, and summation by parts. Applying Cauchy-Schwarz and Hölder we obtain

$$\begin{aligned}\sum_{x\in V}\mu(x)g(x)(f-P_tf)(x) &\leq \int_0^t \sum_{x\in V}\mu(x)|\nabla P_s g|(x)|\nabla f|(x)ds \\ &\leq \int_0^t \||\nabla P_s g|\|_\infty \||\nabla f|\|_1 ds.\end{aligned}$$

Applying (7.17) yields

$$\begin{aligned}(7.19)\quad &\sum_{x\in V}\mu(x)g(x)(f-P_tf)(x) \\ &\leq \int_0^t \sqrt{\frac{12c}{1-\alpha}}\frac{1}{\sqrt{s}}\|g\|_\infty\||\nabla f|\|_1 ds \leq 4\sqrt{\frac{3c}{1-\alpha}}\|g\|_\infty\||\nabla f|\|_1\sqrt{t}.\end{aligned}$$

Now assume for the moment that $\sum_{x\in V}\mu(x)(f-P_tf)(x) \geq 0$. We choose $g = \operatorname{sgn}(f-P_tf)+1+\epsilon$ for some $\epsilon > 0$ such that g is positive and

$$\begin{aligned}\|f-P_tf\|_1 &\leq \sum_{x\in V}\mu(x)|f-P_tf|(x) + (1+\epsilon)\sum_{x\in V}\mu(x)(f-P_tf)(x) \\ &= \sum_{x\in V}\mu(x)g(x)(f-P_tf)(x) \leq (1+\epsilon)8\sqrt{\frac{3c}{1-\alpha}}\||\nabla f|\|_1\sqrt{t}\end{aligned}$$

where we used (7.19) and $\|g\|_\infty = 2$. Taking $\epsilon \to 0$ completes the proof. If $\sum_{x\in V}\mu(x)\cdot(f-P_tf)(x) < 0$ then we choose $g = \operatorname{sgn}(P_tf-f)+1+\epsilon$ and the proof is completed in the same way as above. q.e.d.

With these preparations we can now prove Theorem 7.9.

Proof of Theorem 7.9. We want to apply Lemma 7.18 to the characteristic function χ_U of any subset U. The left hand side becomes

$$\begin{aligned}(7.20)\quad &8\sqrt{\frac{3c}{1-\alpha}}\||\nabla\chi_U|\|_1\sqrt{t} \\ &= 8\sqrt{\frac{3c}{1-\alpha}}\sqrt{t}\sum_{x\in V}\mu(x)\sqrt{\frac{1}{2\mu(x)}\sum_{y\sim x}w_{xy}(\chi_U(y)-\chi_U(x))^2} \\ &\leq 8\sqrt{\frac{3c}{1-\alpha}}\sqrt{t}\sum_{x\in V}\sqrt{\frac{\mu(x)}{2}}\sum_{y\sim x}\sqrt{w_{xy}}|\chi_U(y)-\chi_U(x)| \\ &\leq 8\sqrt{\frac{3c}{1-\alpha}}\sqrt{t}\sum_{x\in V}\sqrt{\frac{\mu(x)}{2w_{\min}}}\sum_{y\sim x}w_{xy}|\chi_U(y)-\chi_U(x)| \\ &\leq 8\sqrt{\frac{3c}{1-\alpha}}\sqrt{t}\sqrt{\frac{2\mu_{\max}}{w_{\min}}}|\partial U|\end{aligned}$$

where $\mu_{\max} = \max_{x\in V} \mu(x)$.

The right hand side becomes:

$$\begin{aligned}
&\|\chi_U - P_t\chi_U\|_1 \\
&= \sum_{x\in U} \mu(x)|\chi_U(x) - P_t\chi_U(x)| + \sum_{x\in V\setminus U} \mu(x)|\chi_U(x) - P_t\chi_U(x)| \\
&\quad = \sum_{x\in U} \mu(x)(1 - P_t\chi_U(x)) + \sum_{x\in V\setminus U} \mu(x)P_t\chi_U(x) \\
&\qquad = 2(\mathrm{vol}(U) - \sum_{x\in U} \mu(x)P_t\chi_U(x)) \\
&\qquad\qquad = 2(\|\chi_U\|_2^2 - \|P_{t/2}\chi_U\|_2^2)
\end{aligned}$$

where we used that $P_{\frac{t}{2}}P_{\frac{t}{2}} = P_t$, $P_t\chi_U \leq 1$, vol(U) $= \sum_{x\in U} \mu(x)P_t\chi_U(x)$ $+ \sum_{x\in V\setminus U} \mu(x)P_t\chi_U(x)$ and the fact that P_t is self-adjoint. Let $\{\psi_i\}_{i=0}^{N-1}$ (N is the number of vertices in the graph) be an orthonormal basis of eigenfunctions, i.e.

$$(\psi_i, \psi_j) = \sum_{x\in V} \mu(x)\psi_i(x)\psi_j(x) = \delta_{ij}.$$

In particular the eigenfunction corresponding to the trivial eigenvalue $\lambda_0 = 0$ is given by $\psi_0 = \frac{1}{\sqrt{\mathrm{vol}(V)}}$. Then every function $f : V \to \mathbb{R}$ can be expanded in the basis $\{\psi_i\}$, i.e. $f = \sum_{i=0}^{N-1} \alpha_i\psi_i$, where $\alpha_i = (f, \psi_i) = \sum_{x\in V} \mu(x)f(x)\psi_i(x)$. For the characteristic function this gives $\chi_U = \sum_{i=0}^{N-1} \alpha_i\psi_i$ with $\alpha_0 = \sum_{x\in V} \mu(x)\chi_U \frac{1}{\sqrt{\mathrm{vol}(V)}} = \frac{\mathrm{vol}(U)}{\sqrt{\mathrm{vol}(V)}}$. Since the ψ_i form an orthonormal basis we have

$$\|\chi_U\|_2^2 = \sum_{x\in V} \mu(x) \sum_{i=0}^{N-1} \alpha_i^2\psi_i^2(x) = \sum_{i=0}^{N-1} \alpha_i^2 = \mathrm{vol}(U).$$

By the spectral theorem,

$$P_t(\chi_U) = \sum_{i=0}^{N-1} e^{-\lambda_i t}\alpha_i\psi_i$$

and thus

$$\|P_{t/2}\chi_U\|_2^2 = \sum_{i=0}^{N-1} e^{-\lambda_i t}\alpha_i^2 \leq e^{-\lambda_1 t} \sum_{i=1}^{N-1} \alpha_i^2 + \alpha_0^2.$$

Combining everything we obtain

$$(7.21)\quad 2(\|\chi_U\|_2^2 - \|P_{t/2}\chi_U\|_2^2) \geq 2(1-e^{-\lambda_1 t})\sum_{i=1}^{N-1}\alpha_i^2$$
$$= 2(1-e^{-\lambda_1 t})\left(\mathrm{vol}(U) - \frac{\mathrm{vol}(U)^2}{\mathrm{vol}(V)}\right).$$

From now on we choose $t_0 = K^{-1}$. The reason is that for this particular choice the constant c is independent of the curvature bound K. From (7.20) and (7.21) we have for all $0 < t \leq K^{-1}$ and all subsets U of V for which $\mathrm{vol}(U) \leq \frac{1}{2}\mathrm{vol}(V)$

$$\frac{|\partial(U)|}{\mathrm{vol(U)}} \geq \frac{(1-e^{-\lambda_1 t})}{C\sqrt{t}},$$

where

$$C = 8\left(\frac{6c\mu_{\max}}{(1-\alpha)w_{\min}}\right)^{\frac{1}{2}}.$$

Since this is true for every subset $U \subset V$ and $0 < t < K^{-1}$ this implies

$$h \geq \frac{1}{C}\sup_{0<t\leq K^{-1}}\frac{(1-e^{-\lambda_1 t})}{\sqrt{t}}.$$

Now if $\lambda_1 \geq K$, we choose $t = \frac{1}{\lambda_1}$ which yields

$$h \geq \frac{1}{C}(1-\frac{1}{e})\sqrt{\lambda_1} \geq \frac{1}{2C}\sqrt{\lambda_1},$$

while if $\lambda_1 \leq K$ we take $t = K^{-1}$ which yields

$$h \geq \frac{1}{C}\sqrt{K}(1-e^{-\frac{\lambda_1}{K}}) \geq \frac{1}{2C\sqrt{K}}\lambda_1.$$

This yields

$$\lambda_1 \leq \max\{2C\sqrt{K}h, 4C^2h^2\}$$

which completes the proof. q.e.d.

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Department of Mathematics
Harvard University
Cambridge, Massachusetts
E-mail address: fbauer@math.harvard.edu

Department of Mathematics
University of Denver
Denver, Colorado
E-mail address: paul.horn@du.edu

Department of Mathematics
Renmin University of China
Beijing, China
E-mail address: linyong01@ruc.edu.cn

Department of Mathematics
Northeastern University
Boston, Massachusetts
E-mail address: g.lippner@neu.edu

Department of Mathematics
Hebrew University
Jerusalem, Israel
E-mail address: mangoubi@math.huji.ac.il

Department of Mathematics
Harvard University
Cambridge, Massachusetts
E-mail address: yau@math.harvard.edu