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Volume doubling, Poincaré inequality and Gaussian heat kernel estimate for non-negatively curved graphs

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Abstract. Studying the heat semigroup, we prove Li–Yau-type estimates for bounded and positive solutions of the heat equation on graphs. These are proved under the assumption of the curvature-dimension inequality $\mathrm{CDE}'(n,0)$, which can be considered as a notion of curvature for graphs. We further show that non-negatively curved graphs (that is, graphs satisfying $\mathrm{CDE}'(n,0)$) also satisfy the volume doubling property. From this we prove a Gaussian estimate for the heat kernel, along with Poincaré and Harnack inequalities. As a consequence, we obtain that the dimension of the space of harmonic functions on graphs with polynomial growth is finite. In the Riemannian setting, this was originally a conjecture of Yau, which was proved in that context by Colding and Minicozzi. Under the assumption that a graph has positive curvature, we derive a Bonnet–Myers-type theorem. That is, we show the diameter of positively curved graphs is finite and bounded above in terms of the positive curvature. This is accomplished by proving some logarithmic Sobolev inequalities.

1. Introduction

The Li–Yau inequality is a very powerful tool for studying positive solutions to the heat equation on manifolds. In its simplest case, it states that a positive solution u (that is, a positive u satisfying $\partial_t u = \Delta u$) on a compact n-dimensional manifold with non-negative curvature satisfies

$$\frac{|\nabla u|^2}{u^2} - \frac{\partial_t u}{u} \le \frac{n}{2t}. \tag{1.1}$$

Beyond its utility in the study of Riemannian manifolds, variants of the Li–Yau inequality have proven to be an important tool in non-Riemannian settings as well. Recently, in [8], the authors proved a discrete version of Li–Yau inequality valid for solutions to the heat equation on

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graphs. The discrete setting provided myriad challenges. Many of these stemmed from the lack of a chain rule for the Laplacian in the graph setting. Overcoming this involved introducing a new notion of curvature for graphs and exploiting crucially the fact that a chain rule formula for the Laplacian does hold in a few isolated cases, along with a discrete version of maximum principle. Indeed, while there are two main methods known to prove the gradient estimate (1.1) – one being the maximum principle (as in [5,31] on manifolds and [32] on graphs), and the other being semigroup methods ([4, 7] on manifolds) – the standard application of both techniques relies heavily on the chain rule and the continuous nature of the underlying space.

The Li–Yau inequality has many applications in Riemannian geometry, but among the most important of these is establishing Harnack inequalities. Indeed, inequality (1.1) can be integrated over space-time in order to derive a Harnack inequality of the form

$$u(x, s) \le C(x, y, s, t)u(y, t), \tag{1.2}$$

where $C(x, y, s, t)$ depends only on the distance of (x, s) and (y, t) in space-time. The Li–Yau inequality, and more generally parabolic Harnack inequalities like (1.2), can also be used to derive further heat kernel estimates. In this direction, one of the most important estimates are Gaussian-type bounds of the following form:

$$\frac{c_l m(y)}{V(x, \sqrt{t})} e^{-C_l \frac{d(x,y)^2}{t}} \le \mathcal{P}_t(x, y) \le \frac{C_r m(y)}{V(x, \sqrt{t})} e^{-c_r \frac{d(x,y)^2}{t}}, \tag{1.3}$$

where $\mathcal{P}_t(x, y)$ is a fundamental solution of the heat equation (heat kernel). The Li–Yau inequality can be used to prove exactly such bounds for the heat kernel on non-negatively curved manifolds. Thus, the Li–Yau inequality implies that non-negatively curved manifolds satisfy a strong form of the Harnack inequality (1.2), along with a Gaussian estimate (1.3). It also is known, by combining the Bishop–Gromov comparison theorem [10] and the work of Buser [11], that non-negatively curved manifolds also satisfy the volume growth condition known as volume doubling and the Poincaré inequality (see also the paper of Grigor'yan, [21]).

In the manifold setting, Grigor'yan [21] and Saloff-Coste [37] independently gave a complete characterization of manifolds satisfying (1.2). They showed that satisfying a volume doubling property along with Poincaré inequalities is actually *equivalent* to satisfying the Harnack inequality (1.2), and is also *equivalent* to satisfying the Gaussian estimate (1.3). Thus, in the manifold setting the three conditions discussed above that are implied by non-negative curvature are actually equivalent. Curvature still plays an important role however, as a local property certifying that a manifold satisfies the three (equivalent) global properties.

In the case of graphs, Delmotte [18] proved a characterization analogous to the one on manifolds discussed above, studying both continuous-time and discrete-time variants of the Gaussian bounds. Until now, however, no known notion of curvature on graphs has been sufficient to imply that a graph satisfies these three conditions. The relationship between these properties and curvature has attracted work in the non-Riemannian case, however. On metric measure spaces, for instance, under some curvature lower bound assumptions, Sturm [39], Rajala [36], Erbar, Kuwada and Sturm [19] and Jiang, Li and Zhang [26] studied the volume doubling property, along with Poincaré inequalities and Gaussian heat kernel estimates.

Despite the successes of [8] in establishing a discrete analogue of the Li–Yau inequality, their ultimate result also had some limitations. Most notably, the results of [8] were insufficient to derive the equivalent conditions of volume doubling and Poincaré inequalities, along with Gaussian heat kernel bounds, and the strongest form of a Harnack inequality. This failure arose from the generalization of (1.1) achieved when considering only a positive solution inside a ball of radius R: in the classical case an extra term of the form "$\frac{1}{R^2}$" occurred, but in the graph case in general the authors were only able to prove a result with an extra term of the factor "$\frac{1}{R}$". This difference resulted in only being able to establish weaker bounds on the heat kernel, and polynomial volume growth as opposed to the stronger condition of volume doubling. Ultimately one of the reasons for these weaker implications was the methods used: [8] used maximum principle arguments, and ultimately ran into problems when cutoff functions were needed.

In this paper, we develop a way to apply semigroup techniques in the discrete setting in order to study the heat kernel of graphs with non-negative Ricci curvature. From here, we obtain a family of global gradient estimates for bounded and positive solutions to the heat equation on an infinite graph, mainly by proving the discrete variational inequality, which is an analogue to the theorem of Baudoin and Garofalo [6] in the manifold setting. The curvature notion used, as in [8], is a modification of the so-called curvature dimension inequality. Satisfying a curvature dimension inequality has proven to be an important generalization of having a Ricci curvature lower bound in the non-Riemannian setting (see, e.g., [2, 4]). The classical curvature dimension inequality however seems weaker when the Laplace operator involved does not satisfy a chain rule. This led to the modification used in this paper (and in [8]) the so-called *exponential curvature dimension inequalities*. A more detailed description of the curvature notion used in this paper, and the motivation behind it, is given in Section 2.2. We note that in the Riemannian case (and more generally when the Laplacian generates a diffusive semigroup) the classical curvature dimension inequality, and the exponential curvature dimension inequalities are equivalent.

From our new methods, we show that non-negatively curved graphs (in the sense of the exponential curvature dimension inequalities) satisfy volume doubling. This improves the results of [8], which only derives polynomial volume growth. We use volume doubling to establish discrete-time Gaussian lower and upper estimates of the heat kernel and ultimately to establish the Poincaré inequality and a Harnack inequality.

As an important technical point, we do not simply establish volume doubling and a Poincaré inequality, and then apply the results of Delmotte [18] to establish the other (equivalent) properties. Instead, after proving volume doubling we attack the Gaussian bounds directly – using volume doubling along with additional information from our methods to establish the bounds. Once the Gaussian bounds are established, we apply the results of Delmotte then "complete the circle" and establish the remaining desired properties. We emphasize that although a number of notions of curvature for graphs have been introduced (see, e.g., [8, 32]), no previous notion has been shown to imply these properties. In fact, [8] was the first paper to show that a non-negative curvature condition for graphs implied polynomial volume growth.

We further derive a continuous-time Gaussian lower bound on the heat kernel. Continuous-time Gaussian *upper* bounds on the heat kernel on graphs turn out not to hold in general, at least for small t. Work of Davies [16] and Pang [34] obtained non-Gaussian upper and lower bounds for the heat kernel on one-dimensional lattice graphs (cf. [34, Theorem 3.5]). They show, for small t, lower bounds that are much larger than the Gaussian bounds would predict.

While our results hold for any non-negatively curved graphs, it is important to note that Gaussian estimates for the heat kernel for Cayley graphs of a finitely generated group of polynomial growth were proved by Hebisch and Saloff-Coste in [24]. For non-uniform transition case, Strook and Zheng proved related Gaussian estimates on lattices in [38].

Establishing that a graph satisfies both volume doubling and the Poincaré inequality has important consequences. For example, under these assumptions on graphs, Delmotte in [17] proved that the dimension of the space of harmonic functions on graphs with polynomial growth is finite. This is an analogue of a similar result on Riemannian manifolds by Colding and Minicozzi from [13], see also Li in [30]. The original problem came from a conjecture of Yau ([42]) which stated for Riemannian manifolds with non-negative Ricci curvature these spaces should be finite dimensional. Thus, our result answers the graph theoretical analogue of Yau's conjecture in the affirmative.

Finally, under the assumption that a graph is positively curved (again, with respect to the exponential curvature dimension inequality), we derive a Bonnet–Myers-type theorem that the diameter of graphs in terms of the canonical distance is finite. We accomplish this by proving certain logarithmic Sobolev inequalities. Here we establish that certain diameter bounds of Bakry ([3]) still hold, even though the Laplacian on graphs does not satisfy the diffusion property that Bakry used. Under the same assumption, we show that the diameter of graphs in terms of graph distance (as opposed to the canonical distance) is also finite. This is done by proving finiteness of measure, and using volume doubling.

The paper is organized as follows: We introduce our notation and formally state our main results in Section 2. In Section 3, we prove our main variational inequality. This inequality leads to a different proof of the Li–Yau gradient estimates on graphs from the one given in [8]. From this main inequality we establish an additional exponential integrability result, and ultimately, volume doubling in Section 4. From volume doubling, we can prove the Gaussian heat kernel estimate, parabolic Harnack inequality and Poincaré inequality in Section 5. Finally, in Section 6, we prove a Bonnet–Myers-type theorem on graphs.

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2. Preliminaries and statement of main results

In this section we develop the preliminaries needed to state our main results. Through the paper, we let $G = (V, E)$ be a finite or infinite connected graph. We allow the edges on the graph to be weighted. Weights are given by a function $\omega : V \times V \to [0, \infty)$; the edge xy from x to y has weight $\omega_{xy} > 0$. In this paper, we assume this weight function is symmetric (that is, $\omega_{xy} = \omega_{yx}$). Furthermore, we assume that

$$\omega_{\min} = \inf_{e \in E, \omega_e > 0} \omega_e > 0.$$

We furthermore allow loops, so it is permissible for $x \sim x$ (and hence $\omega_{xx} > 0$.) Finally, we restrict our interest to the locally finite graphs. That is, we assume that

$$m(x) := \sum_{y \sim x} \omega_{xy} < \infty \quad \text{for all } x \in V.$$

For our work, especially in the context of deriving Gaussian heat kernel bounds, one additional technical assumption is needed. This is essentially needed to compare the continuous time and discrete time heat kernels. In order for the comparison to work smoothly, we need two requirements: First, no edge can be too "small" (this is essentially the content of our assumption $\omega_{\min} > 0$). Second, at each vertex there must be a loop. That is, we must assume $x \sim x$ – this prevents "parity problems" of bipartiteness that would make the continuous and discrete time kernels incomparable. This condition is neatly captured in the following $\Delta(\alpha)$ used by Delmotte in [18], but has also been used previously by other authors.

Definition 2.1. Let $\alpha > 0$. G satisfies $\Delta(\alpha)$ if

(1) $x \sim x$ for every $x \in V$, and
(2) if $x, y \in V$, and $x \sim y$, $\omega_{xy} \geq \alpha m(x)$.

As a remark, if a loop is on every edge and $\sup_x m(x) < \infty$, then the condition $\omega_{\min} > 0$ is sufficient to certify that a graph satisfies $\Delta(\omega_{\min}/\sup_x m(x))$. In general, this is a rather mild condition. It is easy to check, for instance, that adding loops does not decrease the curvature for our curvature condition (see Section 2.2 below) nor change many the geometric quantities we seek to understand (e.g., volume growth, and diameter). Thus even graphs without loops may safely be altered to satisfy this condition.

2.1. Laplace operators on graphs. Let $\mu : V \to \mathbb{R}^+$ be a positive measure on the vertices of the G. Let $V^{\mathbb{R}}$ be the space of real-valued functions on V and, for any $1 \leq p < \infty$, let

$$\ell^p(V, \mu) = \left\{ f \in V^{\mathbb{R}} : \sum_{x \in V} \mu(x) |f(x)|^p < \infty \right\}$$

be the set of ℓ^p integrable functions on V with respect to the measure μ. For $p = \infty$, let

$$\ell^\infty(V, \mu) = \left\{ f \in V^{\mathbb{R}} : \sup_{x \in V} |f(x)| < \infty \right\}$$

be the set of bounded functions. For any $f, g \in \ell^2(V, \mu)$, we let

$$\langle f, g \rangle = \sum_{x \in V} \mu(x) f(x) g(x)$$

denote the standard inner product. This makes $\ell^2(V, \mu)$ a Hilbert space. As is usual, we define the ℓ^p norm of $f \in \ell^p(V, \mu)$, $1 \leq p \leq \infty$:

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

We define the μ-Laplacian $\Delta : V^{\mathbb{R}} \to V^{\mathbb{R}}$ on G by, for any $x \in V$,

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

Similar summations occur frequently, so we introduce the following shorthand notation for such an "averaged sum":

$$\widetilde{\sum_{y \sim x}} h(y) = \frac{1}{\mu(x)} \sum_{y \sim x} \omega_{xy} h(y) \quad \text{for all } x \in V.$$

We treat the case of μ-Laplacians quite generally, but the two most natural choices are the case where $\mu(x) = m(x)$ for all $x \in V$, which is the normalized graph Laplacian, and the case $\mu \equiv 1$ which is the standard graph Laplacian. In this paper, we assume

$$\mu_{\max} := \sup_{x \in V} \mu(x) < \infty.$$

Furthermore, we assume

$$D_\mu := \max_{x \in V} \frac{m(x)}{\mu(x)} < \infty.$$

It is easy to check that $D_\mu < \infty$ is equivalent to the Laplace operator Δ being bounded on $\ell^2(V, \mu)$ (see also [23]). The graph is endowed with its natural graph metric $d(x, y)$, i.e. the smallest number of edges of a path between two vertices x and y. We define balls $B(x, r) = \{y \in V : d(x, y) \leq r\}$, and the volume of a subset A of V, $V(A) = \sum_{x \in A} \mu(x)$. We will write $V(x, r)$ for $V(B(x, r))$.

2.2. Curvature dimension inequalities. In order to study curvature of non-Riemannian spaces, it is important to have a definition that captures, in the non-Riemannian setting, many important consequences of curvature from the manifold setting. One way to do this is through the so-called *curvature-dimension inequality* or CD-inequality. An immediate consequence of the well-known Bochner identity is that on any n-dimensional manifold with curvature bounded below by K, any smooth $f : M \to \mathbb{R}$ satisfies

$$\frac{1}{2}\Delta|\nabla f|^2 \geq \langle \nabla f, \nabla \Delta f \rangle + \frac{1}{n}(\Delta f)^2 + K|\nabla f|^2. \tag{2.1}$$

It was an important insight of Bakry and Emery [2] that (2.1) serves as a substitute for a 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, Bakry and Ledoux [4] succeeded to use it to generalize (1.1) to Markov operators on general measure spaces when the operator satisfies a chain rule-type formula.

To formally state this notion in the graph setting, we first introduce some notation.

Definition 2.2. The gradient form Γ, associated with a μ-Laplacian is defined by

$$\begin{aligned} 2\Gamma(f, g)(x) &= (\Delta(f \cdot g) - f \cdot \Delta(g) - \Delta(f) \cdot g)(x) \\ &= \widetilde{\sum_{y \sim x}} (f(y) - f(x))(g(y) - g(x)). \end{aligned}$$

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

Similarly:

Definition 2.3. The iterated gradient form Γ_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 2.4. The graph G satisfies the CD-inequality $\mathrm{CD}(n, K)$ if, for any function f and at every vertex $x \in V(G)$,

$$\Gamma_2(f) \geq \frac{1}{n}(\Delta f)^2 + K\Gamma(f). \tag{2.2}$$

On graphs – where the Laplace operator fails to satisfy the chain rule – satisfying the $\mathrm{CD}(n, 0)$ inequality seems insufficient to prove a generalization of (1.1). None the less, in [8] the authors prove a discrete analogue of the Li–Yau inequality. The curvature notion they use is a modification of the standard curvature notion, which they call the exponential curvature dimension inequality. In reality, the authors of [8] introduce two slightly different curvature conditions, which they call CDE and CDE$'$, both of which we recall below.

Definition 2.5. We say that a graph G satisfies the *exponential curvature dimension inequality* $\mathrm{CDE}(x, n, K)$ if for any positive function $f : V \to \mathbb{R}^+$ such that $\Delta f(x) < 0$, we have

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

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

Definition 2.6. We say that a graph G satisfies the $\mathrm{CDE}'(x, n, K)$ if for any positive function $f : V \to \mathbb{R}^+$, we have

$$\widetilde{\Gamma_2}(f)(x) \geq \frac{1}{n} f(x)^2(\Delta \log f)(x)^2 + K\Gamma(f)(x). \tag{2.3}$$

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

The reason these are known as the *exponential* curvature dimension inequalities is illustrated in [8, Lemma 3.15], which states the following:

Proposition 2.1. *If the semigroup generated by Δ is a diffusion semigroup (e.g., the Laplacian on a manifold), then* $\mathrm{CD}(n, K)$ *and* $\mathrm{CDE}'(n, K)$ *are equivalent.*

To show that $\mathrm{CDE}'(n, K) \Rightarrow \mathrm{CD}(n, K)$, one takes an arbitrary function f, and applies (2.3) to $\exp(f)$ to verify that (2.2) holds. Likewise, to verify that $\mathrm{CD}(n, K) \Rightarrow \mathrm{CDE}'(n, K)$ one takes an arbitrary positive function f, and applies (2.2) to $\log(f)$ to verify (2.3). This equivalence, however, makes strong use of the chain rule, and hence the fact that Δ generates a diffusion semigroup.

Condition $\mathrm{CDE}'(n, K)$ is a stronger condition than $\mathrm{CDE}(n, K)$ as seen in the following.

Remark 1. Condition $\mathrm{CDE}'(n, K)$ implies $\mathrm{CDE}(n, K)$.

Proof. Let $f : V \to \mathbb{R}^+$ be a positive function for which $\Delta f(x) < 0$. Since $\log s \leq s - 1$ for all positive s, we can write

$$\begin{aligned}\Delta \log f(x) &= \widetilde{\sum_{y \sim x}}(\log f(y) - \log f(x)) = \widetilde{\sum_{y \sim x}} \log \frac{f(y)}{f(x)} \\ &\leq \widetilde{\sum_{y \sim x}} \frac{f(y) - f(x)}{f(x)} = \frac{\Delta f(x)}{f(x)} < 0.\end{aligned}$$

Hence squaring everything reverses the above inequality and we get

$$(\triangle f(x))^2 \leq f(x)^2(\triangle \log f(x))^2,$$

and thus $\mathrm{CDE}(x, n, K)$ is satisfied

$$\widetilde{\Gamma_2}(f)(x) \geq \frac{1}{n} f(x)^2(\triangle \log f)(x)^2 + K\Gamma(f)(x) > \frac{1}{n}(\Delta f)(x)^2 + K\Gamma(f)(x). \qquad \square$$

In [8], the $\mathrm{CDE}(n, K)$ inequality is preferred: the $\Delta \log(f)$ term occurring in the CDE' inequality is awkward in the discrete case, the $\mathrm{CDE}(n, K)$ inequality is weaker in general, and the $\mathrm{CDE}(n, K)$ inequality sufficed for proving the Li–Yau inequality.

None the less, as the results in this paper will show, for the purposes of applying semigroup arguments the $\mathrm{CDE}'(n, K)$ inequality is to be preferred. The primary reason for this is the fact that $\mathrm{CDE}'(n, K)$ implies a non-trivial lower bound on $\widetilde{\Gamma}_2(f)$ for a positive function f at *every* point on a graph, as opposed to just the points where $\Delta f < 0$. For maximum principle arguments, restricting to points where $\Delta f < 0$ turns out not to be a major restriction, but in the more global arguments we apply in this paper $\mathrm{CDE}'(n, K)$ appears to be more useful.

We note that, in general, the conditions CDE' and CDE better capture the spirit of a Ricci curvature lower bound for graphs than the classical CD condition. For instance, every graph satisfies $\mathrm{CD}(2, -1)$ – that is, there is an absolute lower bound to the curvature of graphs. On the other hand, a k-regular tree satisfies $\mathrm{CDE}(2, -\frac{k}{2})$ and this negative curvature is (asymptotically) sharp. Thus with the exponential curvature condition, negative curvature is unbounded. This is unique amongst graph curvature notions.

Moreover, [8] showed that lattices, and more generally Ricci-flat graphs in the sense of Chung and Yau [12] which include the abelian Cayley graphs, have non-negative curvature $\mathrm{CDE}(n, 0)$ and $\mathrm{CDE}'(n, 0)$. Note that $\mathrm{CDE}'(n, K)$ satisfies a product property (cf. the similar result for $\mathrm{CD}(n, K)$ in [33]). As a result, one can construct many graphs satisfying the $\mathrm{CDE}'(n, 0)$ assumption with different dimensions n by taking the Cartesian product of graphs satisfying $\mathrm{CDE}'(n, 0)$.

2.3. Main results. The first main result, alluded to in the introduction, is that satisfying $\mathrm{CDE}'(n, 0)$ is sufficient to imply that a graph satisfies several important conditions: volume doubling, the Poincaré inequality, Gaussian bounds for the heat kernel, and the continuous-time Harnack inequality. For preciseness, we state these conditions now:

Definition 2.7. Let G be a graph.

(DV) The graph G satisfies the *volume doubling* property $\mathrm{DV}(C)$ for a constant $C > 0$ if for all $x \in V$ and all $r > 0$,

$$V(x, 2r) \leq C\, V(x, r).$$

(P) The graph G satisfies the *Poincaré inequality* $\mathrm{P}(C)$ for a constant $C > 0$ if

$$\sum_{x \in B(x_0, r)} m(x)|f(x) - f_B|^2 \leq C r^2 \sum_{x,y \in B(x_0, 2r)} \omega_{xy}(f(y) - f(x))^2$$

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

$$f_B = \frac{1}{V(x_0, r)} \sum_{x \in B(x_0, r)} m(x) f(x).$$

($\mathcal{H}$) Fix $\eta \in (0,1)$ and $0 < \theta_1 < \theta_2 < \theta_3 < \theta_4$ and $C > 0$. The graph G satisfies the *continuous-time Harnack inequality* $\mathcal{H}(\eta, \theta_1, \theta_2, \theta_3, \theta_4, C)$, if for all $x_0 \in V$ and $s, R \in \mathbb{R}^+$, and every positive solution $u(t,x)$ to the heat equation on $Q = [s, s+\theta_4 R^2] \times B(x_0, R)$, we have

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

where

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

(H) Fix $\eta \in (0,1)$ and $0 < \theta_1 < \theta_2 < \theta_3 < \theta_4$ and $C > 0$. The graph G satisfies the *discrete-time Harnack inequality* $\mathrm{H}(\eta, \theta_1, \theta_2, \theta_3, \theta_4, C)$ 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 $Q = ([s, s+\theta_4 R^2] \cap \mathbb{Z}) \times B(x_0, R)$, we have

$$(n^-, x^-) \in Q^-, \quad (n^+, x^+) \in Q^+, \quad d(x^-, x^+) \le n^+ - n^-$$

implies

$$u(n^-, x^-) \le C u(n^+, x^+),$$

where

$$Q^- = ([s + \theta_1 R^2, s + \theta_2 R^2] \cap \mathbb{Z}) \times B(x_0, \eta R),$$
$$Q^+ = ([s + \theta_3 R^2, s + \theta_4 R^2] \cap \mathbb{Z}) \times B(x_0, \eta R).$$

(G) Fix positive constants $c_l, C_l, C_r, c_r > 0$. The graph G satisfies the *Gaussian estimate* $\mathrm{G}(c_l, C_l, C_r, c_r)$ if, whenever $d(x,y) \le n$,

$$\frac{c_l m(y)}{V(x, \sqrt{n})} e^{-C_l \frac{d(x,y)^2}{n}} \le p_n(x,y) \le \frac{C_r m(y)}{V(x, \sqrt{n})} e^{-c_r \frac{d(x,y)^2}{n}}.$$

The first main result of this paper is the following.

Theorem 2.2 (cf. Theorem 5.5). *Suppose that G is a locally finite graph satisfying* $\mathrm{CDE}'(n_0, 0)$ *and* $\Delta(\alpha)$. *Then G has the following four properties.*

(1) *There exist $C_1, C_2, \alpha > 0$ such that* $\mathrm{DV}(C_1)$, $\mathrm{P}(C_2)$, *and* $\Delta(\alpha)$ *are true.*

(2) *There exist $c_l, C_l, C_r, c_r > 0$ such that* $\mathrm{G}(c_l, C_l, C_r, c_r)$ *is true.*

(3) *For any $\eta \in (0,1)$ and $0 < \theta_1 < \theta_2 < \theta_3 < \theta_4$, there exists a constant C_H such that* $\mathrm{H}(\eta, \theta_1, \theta_2, \theta_3, \theta_4, C_H)$ *is true.*

(3)' *For any $\eta \in (0,1)$ and $0 < \theta_1 < \theta_2 < \theta_3 < \theta_4$, there exists a constant $C_{\mathcal{H}}$ such that* $\mathcal{H}(\eta, \theta_1, \theta_2, \theta_3, \theta_4, C_{\mathcal{H}})$ *is true.*

A function u on $V(G)$ is *harmonic* if $\Delta u = 0$. A harmonic function u on G has polynomial growth if there is positive number d such that there exist $x_0 \in V$ and $C > 0$ such that for all $x \in V$,

$$|u(x)| \le C d(x_0, x)^d.$$

Combining Theorem 2.2 and [17, Theorem 3.2], we establish the following graph theoretical analogue of a conjecture of Yau ([42]).

Theorem 2.3. *Suppose that G is a locally finite graph satisfying* $\mathrm{CDE}'(n_0, 0)$ *and* $\Delta(\alpha)$. *Then the dimension of the space of harmonic functions on G having polynomial growth is finite.*

Finally, we prove the following Bonnet–Myers theorems for graphs. We defer the definition of canonical distance of graphs until Section 6.

Theorem 2.4 (cf. Theorem 6.8 and Theorem 6.10). *Suppose that $G = (V, E)$ is a locally finite, connected graph satisfying* $\mathrm{CDE}'(n, K)$ *for some $K > 0$. Then the diameter $\widetilde{D}$ of graph G in terms of the canonical distance is bounded by*

$$\widetilde{D} \leq 4\sqrt{3}\pi\sqrt{\frac{n}{K}},$$

and in particular is finite. Furthermore the diameter D of graph G in terms of the graph distance is also finite, and satisfies

$$D \leq 2\pi\sqrt{\frac{6D_\mu n}{K}}.$$

3. A variational inequality, and Li–Yau-type estimates

In this section we establish our main variational inequality which we develop in order to apply semigroup theoretic arguments in the non-diffusive graph case. This is the content of Section 3.2. An immediate application of this variational inequality is a family of Li–Yau-type inequalities which we derive in Section 3.3.

3.1. The heat kernel on graphs.

3.1.1. The heat equation. A function $u : [0, \infty) \times V \to \mathbb{R}$ is a positive solution to the *heat equation* on $G = (V, E)$ if $u > 0$ and u satisfies the differential equation

$$\Delta u = \partial_t u$$

at every $x \in V$.

In this paper we are primarily interested in the *heat kernel*, that is, the fundamental solutions $p_t(x, y)$ of the heat equation. These are defined so that for any bounded initial condition $u_0 : V \to \mathbb{R}$, the function

$$u(t, x) = \sum_{y \in V} \mu(y) p_t(x, y) u_0(y), \quad t > 0,\ x \in V,$$

satisfies the heat equation, and

$$\lim_{t \to 0^+} u(t, x) = u_0(x).$$

For any subset $U \subset V$, we denote by $\mathring{U} = \{x \in U : \text{for all } y \sim x,\ y \in U\}$ the interior of U. The boundary of U is $\partial U = U \setminus \mathring{U}$. We make use of the following version of the maximum principle.

Lemma 3.1. *Let $U \subset V$ be finite and $T > 0$, and assume that $u : [0, T] \times U \to \mathbb{R}$ is differentiable with respect to the first component and satisfies the inequality*

$$\partial_t u \leq \Delta u$$

on $[0, T] \times \mathring{U}$. Then u attains its maximum on the parabolic boundary

$$\partial_P([0, T] \times U) = (\{0\} \times U) \cup ([0, T] \times \partial U).$$

Proof. Suppose that u attains its maximum at a point $(t_0, x_0) \in (0, T] \times \mathring{U}$ such that

$$\partial_t u(t_0, x_0) < \Delta u(t_0, x_0) \tag{3.1}$$

Then

$$0 \leq \partial_t u(t_0, x_0) < \Delta u(t_0, x_0) = \widetilde{\sum_{y \sim x_0}} (u(t_0, y) - u(t_0, x_0)), \tag{3.2}$$

contradicting the maximality of u.

Otherwise, if at all $(t_0, x_0) \in (0, T] \times \mathring{U}$ which are maximum points at u, there is equality in (3.1) we are done unless there is also equality in (3.2). But this implies that u is constant on $(0, T] \times U$, and hence there is a maximum point on the boundary as desired. □

3.1.2. The heat equation an a domain. Suppose that $U \subset V$ is a finite subset of the vertex set of a graph. We consider the Dirichlet problem (DP),

$$\begin{cases} \partial_t u(t, x) - \Delta_U u(t, x) = 0, & x \in \mathring{U}, t > 0, \\ u(0, x) = u_0(x), & x \in \mathring{U}, \\ u|_{[0,\infty) \times \partial U} = 0. \end{cases}$$

where $\Delta_U : \ell^2(\mathring{U}, \mu) \to \ell^2(\mathring{U}, \mu)$ denotes the Dirichlet Laplacian on $\mathring{U}$.

Note that $-\Delta_U$ is positive and self-adjoint, and $n := \dim \ell^2(\mathring{U}, \mu) < \infty$. Thus the operator $-\Delta_U$ has eigenvalues $0 < \lambda_1 \leq \lambda_2 < \cdots \leq \lambda_n$, along with an orthonormal set of eigenvectors ϕ_i. Here the orthonormality is with respect to the inner product with respect to the measure μ, i.e.

$$\langle \phi_i, \phi_j \rangle = \sum_{x \in V} \mu(x) \phi_i(x) \phi_j(x).$$

The operator Δ_U is a generator of the heat semigroup $P_{t,U} = e^{t\Delta_U}$, $t > 0$. Finite-dimensionality makes the fact that $e^{t\Delta_U} \phi_i = e^{-t\lambda_i} \phi_i$ transparent. The heat kernel $p_U(t, x, y)$ for the finite subset U is then given by

$$p_U(t, x, y) = P_{t,U} \frac{\delta_y}{\sqrt{\mu(y)}}(x) \quad \text{for all } x, y \in \mathring{U},$$

where

$$\delta_y(x) = \sum_{i=1}^{n} \langle \phi_i, \delta_y \rangle \phi_i(x) = \sum_{i=1}^{n} \phi_i(x) \phi_i(y) \sqrt{\mu(y)}.$$

The heat kernel satisfies

$$p_U(t, x, y) = \sum_{i=1}^{n} e^{-\lambda_i t} \phi_i(x) \phi_i(y) \quad \text{for all } x, y \in \mathring{U}.$$

3.1.3. Heat equation on an infinite graph. The heat kernel for an infinite graph can be constructed and its basic properties can be derived using the above ideas by taking an *exhaustion* of the graph. An exhaustion of G is a sequence (U_k) of subsets of V such that $U_k \subset \overset{\circ}{U}_{k+1}$ and $\bigcup_{k\in\mathbb{N}} U_k = V$. For any connected, countable graph G such a sequence exists. One may, for instance, fix a vertex $x_0 \in V$ take the sequence $U_k = B_k(x_0)$ of metric balls of radius k around x_0. The connectedness of our graph G implies that the union of these U_k equals V.

Denoting by p_k, the heat kernel p_{U_k} on U_k, we may extend p_k to all of $(0,\infty) \times V \times V$,

$$p_k(t,x,y) = \begin{cases} p_{U_k}(t,x,y), & x, y \in \overset{\circ}{U}_k, \\ 0, & \text{otherwise.} \end{cases}$$

Then, for any $t > 0$ and $x, y \in V$, we let

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

The maximum principle implies the monotonicity of the heat kernels, i.e. $p_k \le p_{k+1}$, so the above limit exists (but could a priori be infinite). Similarly, it is not a priori clear that p is independent of the exhaustion chosen. Nonetheless, the limit is finite and independent of the exhaustion and p is the desired heat kernel. This construction is carried out in [40] and [41] for unweighted graphs, where the measure $\mu \equiv 1$. For the general case, we refer to [27].

For convenience, we record some important properties of the heat kernel p which we will use in the paper.

Remark 2. For $t, s > 0$ and for all $x, y \in V$, the heat kernel $p(t,x,y)$ satisfies

(1) $p(t,x,y) = p(t,y,x)$,
(2) $p(t,x,y) \ge 0$,
(3) $\sum_{y\in V} \mu(y) p(t,x,y) \le 1$,
(4) $\lim_{t\to 0^+} \sum_{y\in V} \mu(y) p(t,x,y) = 1$,
(5) $\partial_t p(t,x,y) = \Delta_y p(t,x,y) = \Delta_x p(t,x,y)$,
(6) $\sum_{z\in V} \mu(z) p(t,x,z) p(s,z,y) = p(t+s,x,y)$.

From here, the semigroup $P_t : V^{\mathbb{R}} \to V^{\mathbb{R}}$ acting on bounded functions $f : V \to \mathbb{R}$ is as follows. For any bounded function $f \in V^{\mathbb{R}}$,

$$P_t f(x) = \lim_{k\to\infty} \sum_{y\in V} \mu(y) p_k(t,x,y) f(y) = \sum_{y\in V} \mu(y) p(t,x,y) f(y),$$

where $\lim_{t\to 0^+} P_t f(x) = f(x)$. Note that $P_t f(x)$ is a solution of the heat equation. From the properties of the heat kernel, and the boundedness of f, there exists a constant $C > 0$ such that for any $x \in V$, if $\sup_{x\in V} |f(x)| \le C$, then

$$\left| \sum_{y\in V} \mu(y) p(t,x,y) f(y) \right| \le C \lim_{k\to\infty} \sum_{y\in V} \mu(y) p_k(t,x,y) \le C < \infty,$$

so the semigroup is well-defined. The different definitions of the heat semigroup coincide when Δ is a bounded operator or in finite graphs, that is,

$$P_t f(x) = e^{t\Delta} f(x) = \sum_{k=0}^{+\infty} \frac{t^k \Delta^k}{k!} f(x) = \sum_{y\in V} \mu(y) p(t,x,y) f(y).$$

Again we record, without proof, some well-known but useful properties of the semigroup P_t.

Proposition 3.1. *For any bounded function $f, g \in V^{\mathbb{R}}$, and $t, s > 0$, for any $x \in V$, the following statements hold:*

(1) *If $0 \le f(x) \le 1$, then $0 \le P_t f(x) \le 1$.*

(2) $P_t \circ P_s f(x) = P_{t+s} f(x)$.

(3) $\Delta P_t f(x) = P_t \Delta f(x)$.

3.2. The main variational inequality. Finiteness of D_μ implies the operators Δ and Γ are bounded. We in turn derive the following lemma:

Lemma 3.2. *Suppose that G is a (finite or infinite) graph satisfying $\mathrm{CDE}'(n, K)$. Then, for a positive and bounded solution $u(t, x)$ to the heat equation on G, the function $\frac{\Delta u}{2\sqrt{u}}$ on G is bounded at all $t > 0$.*

Proof. The statement is obvious for finite graphs G, so we restrict our attention to infinite graphs.

Fix $R \in \mathbb{N}$ and vertex $x_0 \in V$. We define a cutoff function φ by letting

$$\varphi(x) = \begin{cases} 0, & d(x, x_0) > 2R, \\ \frac{2R - d(x, x_0)}{R}, & R \le d(x, x_0) \le 2R, \\ 1, & d(x, x_0) < R. \end{cases}$$

Let

$$F = \varphi \cdot \frac{\Gamma(\sqrt{u})}{\sqrt{u}}.$$

It is easy to observe that, as $0 \le \varphi(x) \le 1$ for any $x \in V$, $|\Delta\varphi| \le 2D_\mu$. As u is bounded, there exists constants c_1, c_2 so that $0 \le \Gamma(\sqrt{u}) \le c_1$, and $|\Gamma(\Gamma(\sqrt{u}), \varphi)| \le c_2$ as well.

Fix an arbitrary $T > 0$, let (x^*, t^*) be a maximum point of F in $V \times [0, T]$. Clearly, such a maximum exists, as $F \ge 0$ and F is only positive on a bounded region. We may assume $F(x^*, t^*) > 0$. In what follows all computations take place at the point (x^*, t^*). Let $\mathcal{L} = \Delta - \partial_t$, we apply [8, Lemma 4.1] with the choice of $g = \sqrt{u}$. This gives

$$\mathcal{L}(\sqrt{u}F) \le \mathcal{L}(\sqrt{u})F = \left(\Delta(\sqrt{u}) - \frac{\partial_t u}{2\sqrt{u}}\right)F = \frac{2\sqrt{u}\Delta(\sqrt{u}) - \Delta u}{2\sqrt{u}}F = -\frac{F^2}{\varphi}.$$

Further, note that for any $x \in V$,

$$\begin{aligned} \partial_t \Gamma(\sqrt{u})(x) &= \partial_t \frac{1}{2} \widetilde{\sum_{y \sim x}} \left(\sqrt{u}(y) - \sqrt{u}(x)\right)^2 \\ &= \widetilde{\sum_{y \sim x}} (\sqrt{u}(y) - \sqrt{u}(x))(\partial_t \sqrt{u}(y) - \partial_t \sqrt{u}(x)) \\ &= 2\Gamma\left(\sqrt{u}, \frac{\Delta u}{2\sqrt{u}}\right)(x) \end{aligned}$$

yielding

$$\mathcal{L}(\sqrt{u}F) = \mathcal{L}(\varphi \cdot \Gamma(\sqrt{u})) = \Delta\varphi \cdot \Gamma(\sqrt{u}) + 2\Gamma(\Gamma(\sqrt{u}), \varphi) + 2\varphi \cdot \widetilde{\Gamma}_2(\sqrt{u}).$$

Applying the $\mathrm{CDE}'(n, K)$ condition and discarding the $\frac{1}{n}u(\Delta \log \sqrt{u})^2$ term, we obtain

$$-\frac{F^2}{\varphi} \geq \Delta\varphi \cdot \Gamma(\sqrt{u}) + 2\Gamma(\Gamma(\sqrt{u}), \varphi) + 2\varphi K\Gamma(\sqrt{u}).$$

From here, we conclude that

$$F^2(x^*, t^*) \leq 2(D_\mu + |K|)c_1 + c_2,$$

Thus there exists some $C > 0$ so that

$$F(x^*, t^*) \leq C.$$

For $x \in B(x_0, R)$,

$$\frac{\Gamma(\sqrt{u})}{\sqrt{u}}(T, x) = F(x, T) \leq F(x^*, t^*) \leq C.$$

The equation $\Delta u = 2\sqrt{u}\Delta\sqrt{u} + 2\Gamma(\sqrt{u})$ then implies that $\frac{\Delta u}{2\sqrt{u}}$ is bounded at any positive T as well. □

Thus for any bounded function $0 < f \in \ell^\infty(V, \mu)$ on $G(V, E)$, the function $\Gamma(\sqrt{P_{T-t} f})$ is likewise bounded, for any $0 \leq t < T$.

Given a positive bounded f, we let $\phi(t, x)$ be the function

$$\phi(t, x) = P_t(\Gamma(\sqrt{P_{T-t} f}))(x), \quad 0 \leq t < T,\ x \in V.$$

From here we obtain the following (rather crucial) result.

Lemma 3.3. *Suppose that G is a locally finite graph satisfying condition* $\mathrm{CDE}'(n, K)$. *Then, for every $0 \leq t < T$, any $x \in V$, the function ϕ satisfies*

$$\partial_t \phi(t, x) = 2P_t(\widetilde{\Gamma}_2(\sqrt{P_{T-t} f}))(x).$$

Proof. For any $x \in V$,

$$\begin{aligned}
&\partial_t P_t(\Gamma(\sqrt{P_{T-t} f}))(x) \\
&\quad = \partial_t\left(\sum_{y \in V} \mu(y) p(t, x, y)\Gamma(\sqrt{P_{T-t} f})(y)\right) \\
&\quad = \sum_{y \in V} \mu(y)\big(\Delta p(t, x, y)\Gamma(\sqrt{P_{T-t} f})(y) + p(t, x, y)\partial_t\Gamma(\sqrt{P_{T-t} f})(y)\big) \\
&\quad = \sum_{y \in V} \mu(y)\left(\Delta p(t, x, y)\Gamma(\sqrt{P_{T-t} f})(y) - 2p(t, x, y)\Gamma\left(\sqrt{P_{T-t} f}, \frac{\Delta P_{T-t} f}{2\sqrt{P_{T-t} f}}\right)(y)\right) \\
&\quad = \sum_{y \in V} \mu(y) p(t, x, y)\left(\Delta\Gamma(\sqrt{P_{T-t} f})(y) - 2\Gamma\left(\sqrt{P_{T-t} f}, \frac{\Delta P_{T-t} f}{2\sqrt{P_{T-t} f}}\right)(y)\right) \\
&\quad = 2P_t(\widetilde{\Gamma}_2(\sqrt{P_{T-t} f}))(x).
\end{aligned}$$

For the third equality, we observe that for any $x \in V$,

$$\begin{aligned}\partial_t \Gamma(\sqrt{P_{T-t} f})(x) &= \partial_t \frac{1}{2} \widetilde{\sum_{y\sim x}} \big(\sqrt{P_{T-t} f}(y) - \sqrt{P_{T-t} f}(x)\big)^2 \\ &= \widetilde{\sum_{y\sim x}} (\sqrt{P_{T-t} f}(y) - \sqrt{P_{T-t} f}(x))(\partial_t \sqrt{P_{T-t} f}(y) - \partial_t \sqrt{P_{T-t} f}(x)) \\ &= 2\Gamma(\sqrt{P_{T-t} f}, \partial_t \sqrt{P_{T-t} f})(x)\end{aligned}$$

and

$$\partial_t \sqrt{P_{T-t} f} = \frac{\partial_t P_{T-t} f}{2\sqrt{P_{T-t} f}} = -\frac{\Delta P_{T-t} f}{2\sqrt{P_{T-t} f}},$$

where

$$\partial_t P_{T-t} f = -\Delta P_{T-t} f.$$

In the fourth step, note that due to the boundedness of f, the function $\Delta\Gamma(\sqrt{P_{T-t} f})$ is likewise bounded. Similarly from Lemma 3.2, $\Gamma(\sqrt{P_{T-t} f}, \frac{\Delta P_{T-t} f}{2\sqrt{P_{T-t} f}})$ is bounded as well. Then

$$\begin{aligned}&\sum_{y\in V} \mu(y)\bigg(\Delta p(t,x,y)\Gamma(\sqrt{P_{T-t} f})(y) - 2p(t,x,y)\Gamma\bigg(\sqrt{P_{T-t} f}, \frac{\Delta P_{T-t} f}{2\sqrt{P_{T-t} f}}\bigg)(y)\bigg) \\ &\quad= \sum_{y\in V} \mu(y)\Delta p(t,x,y)\Gamma(\sqrt{P_{T-t} f})(y) \\ &\qquad - \sum_{y\in V} \mu(y) 2p(t,x,y)\Gamma\bigg(\sqrt{P_{T-t} f}, \frac{\Delta P_{T-t} f}{2\sqrt{P_{T-t} f}}\bigg)(y) \\ &\quad= \sum_{y\in V} \mu(y) p(t,x,y)\Delta\Gamma(\sqrt{P_{T-t} f})(y) \\ &\qquad - \sum_{y\in V} \mu(y) 2p(t,x,y)\Gamma\bigg(\sqrt{P_{T-t} f}, \frac{\Delta P_{T-t} f}{2\sqrt{P_{T-t} f}}\bigg)(y) \\ &\quad= \sum_{y\in V} \mu(y) p(t,x,y)\bigg(\Delta\Gamma(\sqrt{P_{T-t} f})(y) - 2\Gamma(\sqrt{P_{T-t} f}, \frac{\Delta P_{T-t} f}{2\sqrt{P_{T-t} f}})(y)\bigg),\end{aligned}$$

where various interchanges of sums is justified due to the boundedness of the terms multiplied by the heat kernel (and hence absolute convergence of the sums).

Finally, we justify the exchange of summation and derivation in the second step, which we do by showing the summand converges uniformly on $[0, T]$. To that end, first note the different definitions of the heat semigroup coincide since Δ is a bounded operator. Thus

$$P_t f(x) = e^{t\Delta} f(x) = \sum_{k=0}^{+\infty} \frac{t^k \Delta^k}{k!} f(x) = \sum_{y\in V} \mu(y) p(t,x,y) f(y).$$

Let $\varphi^t(x) = 2\widetilde{\Gamma}_2(\sqrt{P_{T-t} f})(x)$; consider $P_t \varphi^t(x)$ which is the function arising in the summand. As we have shown, there exists a constant $C > 0$ such that $|\varphi^t(x)| \le C$ for any $t \in [0, T]$,

$$|\Delta\varphi^t(x)| = \bigg|\widetilde{\sum_{y\sim x}} (\varphi^t(y) - \varphi^t(x))\bigg| \le 2D_\mu C.$$

Iterating, for any $k \in \mathbb{N}_{\geq 0}$ and $x \in V$,

$$|\Delta^k \varphi^t(x)(x)| \leq 2^k D_\mu^k C.$$

Then

$$\sum_{k=0}^{+\infty} \left| \frac{t^k \Delta^k}{k!} \varphi^t(x) \right| \leq \sum_{k=0}^{+\infty} \frac{T^k}{k!} 2^k D_\mu^k C = Ce^{2D_\mu T} < \infty.$$

Therefore, the series

$$P_t \varphi^t(x) = \sum_{y \in V} \mu(y) p(t,x,y) \varphi^t(y) = \sum_{k=0}^{+\infty} \frac{t^k \Delta^k}{k!} \varphi^t(x)$$

converges uniformly on $[0, T]$, justifying the interchange.

This ends the proof of Lemma 3.3. □

We now obtain some graph theoretical analogues to theorems of Baudoin–Garofalo [6] originating in the manifold setting. In some sense, our main observation is that the $\mathrm{CDE}'(n, K)$ condition can be used in order to overcome the diffusive semigroup assumption usually needed for arguments involving the heat semigroup. This is one of the primary places in this paper where the $\mathrm{CDE}(n, K)$ condition favored in [8] is seemingly insufficient to prove the result.

Theorem 3.2. *Suppose that $G = (V, E)$ is a locally finite, connected graph satisfying $\mathrm{CDE}'(n, K)$. Then, for every positive smooth function $\alpha : [0, T] \to \mathbb{R}^+$, and non-positive smooth function $\gamma : [0, T] \to \mathbb{R}$, every positive and bounded function f satisfies*

$$\partial_t(\alpha\phi) \geq \left(\alpha' - \frac{4\alpha\gamma}{n} + 2\alpha K\right)\phi + \frac{2\alpha\gamma}{n}\Delta P_T f - \frac{2\alpha\gamma^2}{n} P_T f. \tag{3.3}$$

Proof. For any $x \in V$,

$$\begin{aligned}
\partial_t(\alpha\phi)(x) &= \alpha'\phi(x) + 2\alpha P_t(\widetilde{\Gamma}_2(\sqrt{P_{T-t} f}))(x) \\
&\geq \alpha'\phi(x) + 2\alpha P_t\left(\frac{1}{n}\left(\sqrt{P_{T-t} f}\,\Delta \log \sqrt{P_{T-t} f}\right)^2 + K\Gamma(\sqrt{P_{T-t} f})\right)(x) \\
&\geq (\alpha' + 2\alpha K)\phi(x) + 2\alpha \sum_{\substack{y\sim x \\ \Delta\sqrt{P_{T-t} f}(y) < 0}} \mu(y) p(t,x,y) \frac{1}{n}\left(\Delta\sqrt{P_{T-t} f}\right)^2(y) \\
&\quad + 2\alpha \sum_{\substack{y\sim x \\ \Delta\sqrt{P_{T-t} f}(y) \geq 0}} \mu(y) p(t,x,y) \frac{1}{n}\left(\sqrt{P_{T-t} f}\,\Delta \log \sqrt{P_{T-t} f}\right)^2(y) \\
&\geq (\alpha' + 2\alpha K)\phi(x) + \frac{2\alpha}{n} P_t(\gamma\Delta P_{T-t} f - 2\gamma\Gamma(\sqrt{P_{T-t} f}) - \gamma^2 P_{T-t} f)(x) \\
&= (\alpha' + 2\alpha K)\phi(x) + \frac{2\alpha\gamma}{n} P_t(\Delta P_{T-t} f)(x) - \frac{4\alpha\gamma}{n} P_t(\Gamma(\sqrt{P_{T-t} f}))(x) \\
&\quad - \frac{2\alpha\gamma^2}{n} P_t(P_{T-t} f)(x) \\
&= \left(\alpha' - \frac{4\alpha\gamma}{n} + 2\alpha K\right)\phi(x) + \frac{2\alpha\gamma}{n}\Delta P_T f(x) - \frac{2\alpha\gamma^2}{n} P_T f(x).
\end{aligned}$$

The first inequality in the above proof comes from applying the $\mathrm{CDE}'(n, K)$ inequality to the function $\sqrt{P_{T-t} f}$. The second one comes from Jensen's inequality, under the assumption that $(\Delta\sqrt{P_{T-t} f})(y) < 0$. This is essentially the contents of Remark 1 – really we apply the $\mathrm{CDE}(n, K)$ inequality at points so that $\Delta\sqrt{P_{T-t} f}(y) < 0$.

The third inequality is a bit more subtle and is derived as follows: Clearly, for any function γ, one has

$$(\Delta\sqrt{P_{T-t} f})(y)^2 \geq 2\gamma\sqrt{P_{T-t} f}(y)\Delta\sqrt{P_{T-t} f}(y) - \gamma^2 P_{T-t} f(y).$$

Since γ is non-positive, if $\Delta\sqrt{P_{T-t} f}(y) \geq 0$, the right-hand of the above inequality is also non-positive. Thus in this case it is also true that

$$\big(\sqrt{P_{T-t} f}\,\Delta \log\sqrt{P_{T-t} f}\big)^2(y) \geq 2\gamma\sqrt{P_{T-t} f}(y)\Delta\sqrt{P_{T-t} f}(y) - \gamma^2 P_{T-t} f(y),$$

as the left-hand side of this inequality is clearly non-negative. Furthermore, by the identity

$$\Delta u = 2\sqrt{u}\Delta\sqrt{u} + 2\Gamma(u),$$

one has

$$2\sqrt{P_{T-t} f}\,\Delta\sqrt{P_{T-t} f} = \Delta P_{T-t} f - 2\Gamma(\sqrt{P_{T-t} f}),$$

Therefore,

$$\begin{aligned}\sum_{\substack{y\sim x\\ \Delta\sqrt{P_{T-t} f}(y)<0}} &\mu(y)p(t,x,y)\big(\Delta\sqrt{P_{T-t} f}\big)^2(y)\\ &+ \sum_{\substack{y\sim x\\ \Delta\sqrt{P_{T-t} f}(y)\geq 0}} \mu(y)p(t,x,y)P_{T-t} f(y)\big(\Delta \log\sqrt{P_{T-t} f}\big)^2(y)\\ &\geq P_t(\gamma\Delta P_{T-t} f - 2\gamma\Gamma(\sqrt{P_{T-t} f}) - \gamma^2 P_{T-t} f)(x),\end{aligned}$$

as desired. □

3.3. Li–Yau inequalities. The power of Theorem 3.2 is, perhaps, a bit hard to appreciate at first. As an application, it can be used to give an alternative derivation of the Li–Yau inequality. Indeed, it can be used to derive a *family* of similar differential Harnack inequalities. The key in applying Theorem 3.2 is to choose γ so that a nice simplification occurs.

For instance, suppose that for some (smooth) function α we choose γ in such a way that

$$\alpha' - \frac{4\alpha\gamma}{n} + 2\alpha K = 0.$$

That is, choose

$$\gamma = \frac{n}{4}\left(\frac{\alpha'}{\alpha} + 2K\right).$$

If α is chosen appropriately to make γ non-positive, then integrating inequality (3.3) obtained in Theorem 3.2 from 0 to T yields an estimate. Setting $W = \sqrt{\alpha}$, one obtains the following result.

Theorem 3.3. *Suppose that $G = (V, E)$ is a locally finite and connected graph satisfying $\mathrm{CDE}'(n, K)$, and let $W : [0, T] \to \mathbb{R}^+$ be a smooth function such that*

$$W(0) = 1, W(T) = 0,$$

and so that

$$W'(t) \leq -KW(t)$$

for $0 \leq t \leq T$. Then, for any bounded and positive function $f \in V^{\mathbb{R}}$,

$$\frac{\Gamma(\sqrt{P_T f})}{P_T f} \leq \frac{1}{2}\left(1 - 2K\int_0^T W(s)^2\,ds\right)\frac{\Delta P_T f}{P_T f} + \frac{n}{2}\left(\int_0^T W'(s)^2\,ds + K^2\int_0^T W(s)^2\,ds - K\right). \tag{3.4}$$

Here, the condition $W' \leq -KW$ amounts to the non-positivity of γ. As observed in [6], the family obtained by taking

$$W(t) = \left(1 - \frac{t}{T}\right)^b$$

for any $b > \frac{1}{2}$ is quite interesting in the region where $-\frac{b}{T} < K$. For this family,

$$\int_0^T W(s)^2\,ds = \frac{T}{2b+1}$$

and

$$\int_0^T W'(s)^2\,ds = \frac{b^2}{(2b-1)T}.$$

Thus for such a choice of W, estimate (3.4) yields

$$\frac{\Gamma(\sqrt{P_T f})}{P_T f} \leq \frac{1}{2}\left(1 - \frac{2KT}{2b+1}\right)\frac{\Delta P_T f}{P_T f} + \frac{n}{2}\left(\frac{b^2}{(2b-1)T} + \frac{K^2 T}{2b+1} - K\right). \tag{3.5}$$

When $K = 0$ and $b = 1$, this reduces to the familiar Li–Yau inequality on graphs (as derived by [8]). Indeed, per the identity $\Delta P_t f = \partial_t P_t f = 2\sqrt{P_t f}\,\partial_t\sqrt{P_t f}$ and switching the notion T to t, (3.5) reduces to

$$\frac{\Gamma(\sqrt{P_t f})}{P_t f} - \frac{\partial_t\sqrt{P_t f}}{\sqrt{P_t f}} \leq \frac{n}{2t}, \quad t > 0.$$

4. Volume growth

While the Li–Yau inequality is an attractive consequence of Theorem 3.2, a version was already known to hold on graphs using the $\mathrm{CDE}(n, K)$ curvature-dimensional inequality (which is slightly weaker than the $\mathrm{CDE}'(n, K)$ inequality used in Theorem 3.2).

In this section, we begin by exhibiting a further application of the variational inequality, and use it derive volume doubling from non-negative curvature. Establishing volume doubling was out of reach of previous work.

Theorem 4.1. *Let $G = (V, E)$ be a locally finite and connected graph satisfying condition* $\mathrm{CDE}'(n, 0)$. *There exists an absolute positive constant $\rho > 0$, and $A > 0$, depending only on n, such that*

$$P_{Ar^2}(\mathbf{1}_{B(x,r)})(x) \geq \rho, \quad x \in V,\ r > \frac{1}{2}. \tag{4.1}$$

Proof. Again, we proceed by carefully choosing a γ to apply Theorem 3.2. Let

$$\alpha(t) = \tau + T - t, \quad \gamma(t) = -\frac{n}{4(\tau + T - t)}$$

for $\tau > 0$, and $K = 0$. For such a choice

$$\alpha' - \frac{4\alpha\gamma}{n} + 2\alpha K = 0, \quad \frac{2\alpha\gamma}{n} = -\frac{1}{2}, \quad \frac{2\alpha\gamma^2}{n} = \frac{n}{8(\tau + T - t)},$$

after simplifying the main inequality. Integrate the inequality from 0 to T to obtain

$$\tau P_T(\Gamma(\sqrt{f})) - (T + \tau)\Gamma(\sqrt{P_T f}) \geq -\frac{T}{2}\Delta P_T f - \frac{n}{8}\log\left(1 + \frac{T}{\tau}\right) P_T f. \tag{4.2}$$

Now, suppose that f is a non-positive c-Lipschitz function (that is, $|f(y) - f(x)| \leq c$ if $x \sim y$.) Fix $\lambda \geq 0$, and consider the function $\varphi = e^{2\lambda f}$. Clearly, φ is positive and bounded. Let

$$\psi(\lambda, t) = \frac{1}{2\lambda}\log(P_t e^{2\lambda f})$$

so that $P_t\varphi = P_t(e^{2\lambda f}) = e^{2\lambda\psi}$.

Applying (4.2) to φ, and switching notation from T to t, one obtains that

$$\tau P_t(\Gamma(e^{\lambda f})) - (t + \tau)\Gamma(e^{\lambda\psi}) \geq -\frac{t}{2}\Delta P_t\varphi - \frac{n}{8}\log\left(1 + \frac{t}{\tau}\right)e^{2\lambda\psi}. \tag{4.3}$$

Fix $x \in V$. Taking $C(\lambda, c) = \sqrt{\frac{D_\mu}{2}}ce^{\lambda c} < \infty$,

$$\begin{aligned}
\Gamma(e^{\lambda f})(x) &= \frac{1}{2}\widetilde{\sum_{y\sim x}}\left(e^{\lambda f(y)} - e^{\lambda f(x)}\right)^2 \\
&= \frac{1}{2}e^{2\lambda f(x)}\widetilde{\sum_{y\sim x}}\left(e^{\lambda(f(y)-f(x))} - 1\right)^2 \\
&= \frac{1}{2}e^{2\lambda f(x)}\Bigg(\widetilde{\sum_{0\leq f(y)-f(x)\leq c}}\left(e^{\lambda(f(y)-f(x))} - 1\right)^2 \\
&\qquad + \widetilde{\sum_{-c\leq f(y)-f(x)\leq 0}}\left(e^{\lambda(f(y)-f(x))} - 1\right)^2\Bigg) \\
&\leq \frac{1}{2}e^{2\lambda f(x)}\Bigg(e^{2\lambda c}\widetilde{\sum_{0\leq f(y)-f(x)\leq c}}\left(1 - e^{-\lambda c}\right)^2 \\
&\qquad + \widetilde{\sum_{-c\leq f(y)-f(x)\leq 0}}\left(e^{-\lambda c} - 1\right)^2\Bigg) \\
&\leq \frac{1}{2}e^{2\lambda f(x)}e^{2\lambda c}\widetilde{\sum_{y\sim x}}\left(e^{-\lambda c} - 1\right)^2 \\
&\leq C(\lambda, c)^2\lambda^2 e^{2\lambda f(x)}.
\end{aligned}$$

This allows us to upper bound the left-hand side of (4.3), obtaining

$$\tau P_t(\Gamma(e^{\lambda f})) - (t+\tau)\Gamma(e^{\lambda\psi}) \le \tau P_t(\Gamma(e^{\lambda f})) \le C(\lambda,c)^2\lambda^2\tau P_t(e^{2\lambda f}) \\ = C(\lambda,c)^2\lambda^2\tau e^{2\lambda\psi}.$$

Combining this with the fact that

$$\Delta P_t\varphi = \partial_t e^{2\lambda\psi} = 2\lambda e^{2\lambda\psi}\partial_t\psi,$$

we obtain that

$$\partial_t\psi \ge -\frac{\lambda}{t}\left(C(\lambda,c)^2\tau + \frac{n}{8\lambda^2}\log\left(1+\frac{t}{\tau}\right)\right). \tag{4.4}$$

Since (4.4) holds for all τ, we optimize. Set τ to be the optimal value

$$\tau_0 = \frac{t}{2}\left(\sqrt{1+\frac{n}{2\lambda^2 C(\lambda,c)^2 t}}-1\right),$$

and substitute into (4.4) to obtain

$$-\partial_t\psi \le \lambda C(\lambda,c)^2 G\left(\frac{1}{\lambda^2 C(\lambda,c)^2 t}\right). \tag{4.5}$$

Here,

$$G(s) = \frac{1}{2}\left(\sqrt{1+\frac{n}{2}s}-1\right) + \frac{n}{8}s\log\left(1+\frac{2}{\sqrt{1+\frac{n}{2}s}-1}\right), \quad s>0.$$

Note that $G(s)\to 0$ as $s\to 0^+$, and that $G(s)\sim\sqrt{\frac{ns}{2}}$ as $s\to+\infty$. Integrate inequality (4.5) between t_1 and t_2 (for $t_1\le t_2$) to obtain

$$\psi(\lambda,t_1)\le\psi(\lambda,t_2)+\lambda C(\lambda,c)^2\int_{t_1}^{t_2} G\left(\frac{1}{\lambda^2 C(\lambda,c)^2 t}\right)dt.$$

Jensen's inequality in ψ yields that

$$2\lambda\psi(\lambda,t) = \ln(P_t e^{2\lambda f}) \ge P_t(\ln e^{2\lambda f}) = 2\lambda P_t f.$$

This yields that $\lambda P_{t_1} f \le \lambda\psi(\lambda,t_1)$. Combining with the previous inequality shows that for all $t_1\le t_2$,

$$P_{t_1}(\lambda f) \le \lambda\psi(\lambda,t_2) + \lambda^2 C(\lambda,c)^2\int_{t_1}^{t_2} G\left(\frac{1}{\lambda^2 C(\lambda,c)^2 t}\right)dt.$$

Replacing t_2 with t, and letting $t_1\to 0^+$, we obtain

$$\lambda f \le \lambda\psi(\lambda,t) + \lambda^2 C(\lambda,c)^2\int_0^t G\left(\frac{1}{\lambda^2 C(\lambda,c)^2\tau}\right)d\tau. \tag{4.6}$$

Now fix a vertex $x\in V$. Let $B=B(x,r)$, and consider the function $f(y)=-d(y,x)$. Clearly, f is 1-Lipschitz. For such a 1-Lipschitz function, we may use

$$C(\lambda,c) = \sqrt{\frac{D_\mu}{2}}e^\lambda$$

in the proceeding.

Clearly,

$$e^{2\lambda f} \leq e^{-2\lambda r}\mathbf{1}_{B^c} + \mathbf{1}_B.$$

Thus for every $t > 0$ one has

$$e^{2\lambda\psi(\lambda,t)(x)} = P_t(e^{2\lambda f})(x) \leq e^{-2\lambda r} + P_t(\mathbf{1}_B)(x),$$

which yields the lower bound

$$P_t(\mathbf{1}_B)(x) \geq e^{2\lambda\psi(\lambda,t)(x)} - e^{-2\lambda r}.$$

Inequality (4.6) allows us to estimate the first term in this lower bound. If

$$\phi(\lambda C(\lambda,c),t) = \lambda^2 C(\lambda,c)^2 \int_0^t G\left(\frac{1}{\lambda^2 C(\lambda,c)^2\tau}\right) d\tau,$$

then (4.6) yields

$$1 = e^{2\lambda f(x)} \leq e^{2\lambda\psi(\lambda,t)(x)} e^{2\phi(\lambda C(\lambda,c),t)}.$$

Hence

$$P_t(\mathbf{1}_B)(x) \geq e^{-2\phi(\lambda C(\lambda,c),t)} - e^{-2\lambda r}.$$

Choose $\lambda C(\lambda,c) = \frac{1}{r}$, $t = Ar^2$ to obtain

$$P_{Ar^2}(\mathbf{1}_B)(x) \geq e^{-2\phi(\frac{1}{r},Ar^2)} - e^{-\frac{2}{C(\lambda,c)}}.$$

To finish, we must choose $A > 0$ sufficiently small, depending only on n, and a $\rho > 0$ so that for every $x \in V$ and $r > \frac{1}{2}$,

$$e^{-2\phi(\frac{1}{r},Ar^2)} - e^{-\frac{2}{C(\lambda,c)}} \geq \rho. \tag{4.7}$$

(Note that, actually, the point that $r > \frac{1}{2}$ simply implies that the term $e^{-\frac{2}{C(\lambda,c)}}$ is not one. Replacing this by $r > \epsilon$ for any positive ϵ would likewise suffice.)

To see that such an A exists, consider the function

$$\phi\left(\frac{1}{r}, Ar^2\right) = \frac{1}{r^2}\int_0^{Ar^2} G\left(\frac{r^2}{\tau}\right) d\tau = \int_{A^{-1}}^{\infty} \frac{G(t)}{t^2}\, dt.$$

One has $\phi(\frac{1}{r}, Ar^2) \to 0$ as $A \to 0^+$, and hence such a sufficiently small A exists to ensure that (4.7) holds and this completes the proof. □

Now we use the previous result to show that non-negatively curved graphs (with respect to CDE$'$) satisfy the volume doubling property. That is, we prove:

Theorem 4.2. *Suppose that G is a locally finite, connected graph satisfying* $\mathrm{CDE}'(n,0)$. *Then G satisfies the volume doubling property* $\mathrm{DV}(C)$. *That is, there exists a positive constant $C = C(n, D_\mu, \mu_{\max}, \omega_{\min})$ such that for all $x \in V$ and all $r > 0$,*

$$V(x,2r) \leq C\,V(x,r).$$

Actually, some simple computations give slightly stronger conclusions on volume regularity. We will find these useful later, in the proof of a Gaussian estimate.

Remark 3. For any $r \geq s$,

$$\begin{aligned} V(x,r) &\leq V\Big(x, 2^{\left[\frac{\log(\frac{r}{s})}{\log 2}\right]+1} s\Big) \\ &\leq C^{1+\frac{\log(\frac{r}{s})}{\log 2}} V(x,s) \\ &= C\left(\frac{r}{s}\right)^{\frac{\log C}{\log 2}} V(x,s), \end{aligned}$$

where $[x]$ denotes the integer part of x.

One final tool in the proof of Theorem 4.2 is an explicit form of a Harnack inequality arising from the Li–Yau inequality as derived in [8]. In the (simplified by our assumption that $K = 0$) form in which we apply it, it states the following:

Corollary 4.3. *Suppose that G is a finite or infinite graph satisfying* $\mathrm{CDE}'(n, 0)$. *Then, for every $x \in V$ and $(t, y), (s, z) \in (0, +\infty) \times V$ with $t < s$, one has*

$$p(t,x,y) \leq p(s,x,z)\left(\frac{s}{t}\right)^n \exp\left(\frac{4\mu_{\max} d(y,z)^2}{\omega_{\min}(s-t)}\right).$$

We now turn to the proof of Theorem 4.2.

Proof. From the semigroup property and the symmetry of the heat kernel given in Remark 2, for any $y \in V$ and $t > 0$ one has

$$p(2t, y, y) = \sum_{z \in V} \mu(z) p(t, y, z)^2.$$

Consider a cutoff function $h \in V^{\mathbb{R}}$ such that $0 \leq h \leq 1$, $h \equiv 1$ on $B(x, \frac{\sqrt{t}}{2})$ and $h \equiv 0$ outside $B(x, \sqrt{t})$. We have

$$\begin{aligned} P_t h(y) &= \sum_{z \in V} \mu(z) p(t, y, z) h(z) \\ &\leq \left(\sum_{z \in V} \mu(z) p(t, y, z)^2\right)^{\frac{1}{2}} \left(\sum_{z \in V} \mu(z) h(z)^2\right)^{\frac{1}{2}} \\ &\leq (p(2t, y, y))^{\frac{1}{2}} (V(x, \sqrt{t}))^{\frac{1}{2}}. \end{aligned}$$

Take $y = x$, and $t = r^2$ to obtain

$$\big(P_{r^2}(\mathbf{1}_{B(x,\frac{r}{2})})(x)\big)^2 \leq (P_{r^2} h(x))^2 \leq p(2r^2, x, x) V(x, r). \tag{4.8}$$

At this point we use the crucial inequality (4.1), which gives for some $0 < A < 1$, depending on the dimension n,

$$P_{Ar^2}(\mathbf{1}_{B(x,r)})(x) \geq \rho, \quad x \in V,\ r > \frac{1}{2}.$$

Combine the latter inequality with (4.8) and Corollary 4.3 to obtain an on-diagonal lower bound

$$p(2r^2, x, x) \geq \frac{\rho^*}{V(x,r)}, \quad x \in V,\ r > \frac{1}{2}. \tag{4.9}$$

Apply Corollary 4.3 to $p(t,x,y)$, to obtain that for every $y \in B(x,\sqrt{t})$,

$$p(t,x,x) \le C(n,\mu_{\max},\omega_{\min})p(2t,x,y). \tag{4.10}$$

Integrating the above inequality over $B(x,\sqrt{t})$ with respect to y gives

$$p(t,x,x)V(x,\sqrt{t}) \le C \sum_{y\in B(x,\sqrt{t})} \mu(y)p(2t,x,y) \le C.$$

Taking $t = 4r^2$ yields the on-diagonal upper bound

$$p(4r^2,x,x) \le \frac{C}{V(x,2r)}. \tag{4.11}$$

Combining (4.9) and (4.10) with (4.11), we finally obtain for any $r > \frac{1}{2}$,

$$V(x,2r) \le \frac{C}{p(4r^2,x,x)} \le \frac{C^*}{p(2r^2,x,x)} \le C^{**}V(x,r).$$

When $0 < r \le \frac{1}{2}$, $V(x,2r) \equiv V(x,r) = \mu(x)$, the result is obvious. This completes the proof of the corollary. □

As a remark, while the proof is fairly simple, it illustrates the power of inequality (4.8). In [8], polynomial volume growth was proved for non-negatively curved graphs through a direct, but somewhat unusual, application of the Harnack inequality (cf. [8, Corollary 7.5]). A stronger Harnack inequality, of the type introduced in Section 2 and which implies volume doubling, was only proven under the assumption of a "strong cutoff function". Such a function was shown to exist in some cases, but for non-negatively curved graphs in general only a weaker Li–Yau inequality was proved which led to a weaker Harnack inequalities could not imply volume doubling. The lesson here should be taken that *using the heat-semigroup arguments as done above allows us to work around the lack of strong cutoff functions for graphs.*

5. Gaussian estimates

In this section we focus on the normalized Laplacian: that is, we take our measure μ to be $\mu(x) = m(x)$. We will prove a discrete-time Gaussian estimate on an infinite, connected and locally finite graph $G = (V, E)$.

Let $\mathcal{P}_t(x,y) = p(t,x,y)m(y)$ be the continuous-time Markov kernel on the graph. It is also a solution of the heat equation. By symmetry, the heat kernel $p(t,x,y)$ satisfies

$$\frac{\mathcal{P}_t(x,y)}{m(y)} = \frac{\mathcal{P}_t(y,x)}{m(x)}.$$

Let $p_n(x,y)$ be the discrete-time kernel on G, which is defined by

$$\begin{cases} p_0(x,y) = \delta_{xy}, \\ p_{k+1}(x,z) = \sum_{y\in V} p(x,y)p_k(y,z), \end{cases}$$

where $p(x,y) := \frac{\omega_{xy}}{m(x)}$, and $\delta_{xy} = 1$ only when $x = y$, otherwise equals 0. We know the two kernels satisfy

$$e^{-t}\sum_{k=0}^{+\infty}\frac{t^k}{k!}p_k(x,y) = \mathcal{P}_t(x,y). \tag{5.1}$$

In order to obtain our desired Gaussian estimate, we first establish a continuous-time Gaussian on-diagonal estimate for graphs. Work in [8] shows that their Harnack inequality suffices to prove a Gaussian *upper* bound for bounded degree graphs satisfying CDE$(n,0)$. A Gaussian lower bound was not proven, however. This failure is closely tied to the inability to use CDE to imply volume doubling. With the new information gleaned from our modified curvature condition, we *are* however able to derive a Gaussian lower bound, as we now illustrate.

Theorem 5.1. *Suppose that G is a locally finite graph satisfying* CDE$'(n_0,0)$. *Then G satisfies the continuous-time Gaussian estimate. That is, there exists a constant C depending on n_0 so that, for any $x,y \in V$ and for all $t > 0$,*

$$\mathcal{P}_t(x,y) \le \frac{Cm(y)}{V(x,\sqrt{t})}.$$

Furthermore, for any $t_0 > 0$, there exist constants C' and c' so that for all $t > t_0$,

$$\mathcal{P}_t(x,y) \ge \frac{C'm(y)}{V(x,\sqrt{t})}\exp\left(-c'\frac{d(x,y)^2}{t}\right).$$

Proof. The upper bound follows from the methods of [8], as the Harnack inequality obtained in that paper still applies for graphs satisfying CDE$'(n_0,0)$. For completeness, we include the brief proof. From Corollary 4.3, for any $t > 0$, choosing $s = 2t$ and for any $z \in B(x,\sqrt{t})$, we have

$$p(t,x,y) \le p(2t,z,y)2^{n_0}\exp\left(\frac{4\mu_{\max}}{\omega_{\min}}\right).$$

Integrating the above inequality over $B(x,\sqrt{t})$ with respect to z gives

$$p(t,x,y) \le \frac{C}{V(x,\sqrt{t})}\sum_{z\in B(x,\sqrt{t})}\mu(z)p(2t,z,y) \le \frac{C}{V(x,\sqrt{t})}.$$

We now prove the lower bound estimate. Recall that we only claim the result under the assumption that $t > t_0$. The result is most transparent if $t_0 > \frac{1}{2}$. In this case, then taking $t > \frac{1}{2}$ and choosing $2r^2 = \varepsilon t$ for some $0 < \varepsilon < 1$, equation (4.9) implies that every $x \in V$ satisfies

$$p(\varepsilon t,x,x) \ge \frac{\rho^*}{V(x,\sqrt{\frac{\varepsilon t}{2}})} \ge \frac{\rho^*}{V(x,\sqrt{t})}. \tag{5.2}$$

Applying Corollary 4.3, taking εt as "t", taking t to be "s", and choosing $y = x, z = y$, we obtain

$$p(\varepsilon t,x,x) \le p(t,x,y)\varepsilon^{n_0}\exp\left(\frac{4\mu_{\max}d(x,y)^2}{\omega_{\min}(1-\varepsilon)t}\right). \tag{5.3}$$

Combining (5.2) with (5.3), we finally obtain for any $t > \frac{1}{2}$,

$$p(t,x,y) \geq \frac{\varepsilon^{-n_0}\rho^*}{V(x,\sqrt{t})}\exp\left(-\frac{4\mu_{\max}d(x,y)^2}{\omega_{\min}(1-\varepsilon)t}\right) = \frac{C'}{V(x,\sqrt{t})}\exp\left(-c'\frac{d(x,y)^2}{t}\right).$$

While we assumed that $t > \frac{1}{2}$ here, if we fix *any* $t_0 > 0$, it is easy to rework the proof Theorem 4.1 to work with such an arbitrary t_0 and this completes the proof of the theorem. □

The remaining difficulty is verifying that the lower bound holds for small t (as $t \to 0^+$). This we will defer to Remark 4, which we prove after establishing the discrete-time Gaussian estimate. Together, this will complete the proof of Theorem 5.1.

As a special case, note that if $t \geq \max\{d(x,y)^2, \frac{1}{2}\}$, then the lower estimate can be written as

$$p(t,x,y) \geq \frac{C''}{V(x,\sqrt{t})}. \tag{5.4}$$

Before we ultimately finish the continuous-time lower bound, we address the discrete-time estimate. We begin with the on-diagonal estimate:

Proposition 5.2. *Suppose that G is a graph satisfying* $\mathrm{CDE}'(n_0, 0)$ *and* $\Delta(\beta)$. *Then there exist $c_d, C_d > 0$, for any $x, y \in V$, such that*

$$p_n(x,y) \leq \frac{C_d m(y)}{V(x,\sqrt{n})} \quad \textit{for all } n > 0,$$
$$p_n(x,y) \geq \frac{c_d m(y)}{V(x,\sqrt{n})} \quad \textit{if } n \geq d(x,y)^2.$$

This proposition follows the methods of Delmotte from [18]. To prove it, we first introduce some necessary results. Assume that $\Delta(\alpha)$ holds (cf. Definition 2.1), so that we can consider the positive submarkovian kernel

$$\overline{p}(x,y) = p(x,y) - \alpha\delta_{xy}.$$

Now, compute $\mathcal{P}_n(x,y)$ and $p_n(x,y)$ with $\overline{p}(x,y)$,

$$\mathcal{P}_n(x,y) = e^{(\alpha-1)n}\sum_{k=0}^{+\infty}\frac{n^k}{k!}\overline{p}_k(x,y) = \sum_{k=0}^{+\infty} a_k\overline{p}_k(x,y),$$
$$p_n(x,y) = \sum_{k=0}^{n} C_n^k\alpha^{n-k}\overline{p}_k(x,y) = \sum_{k=0}^{n} b_k\overline{p}_k(x,y).$$

There is a lemma from [18] to compare the two sums as follows.

Lemma 5.1. *Let $c_k = \frac{b_k}{a_k}$, for $0 \leq k \leq n$, and suppose $\alpha \leq \frac{1}{4}$. Then the following statements hold:*

- *$c_k \leq C(\alpha)$ when $0 \leq k \leq n$,*
- *$c_k \geq C(a,\alpha) > 0$ when $n \geq \frac{a^2}{\alpha^2}$ and $|k-(1-\alpha)n| \leq a\sqrt{n}$.*

Note that the condition that $\alpha \leq \frac{1}{4}$ implies that $\frac{n}{2} \leq k \leq n$ in the second assertion. Note that assuming $\alpha \leq \frac{1}{4}$ does not inhibit us: it is clear from the definition that if $\Delta(\alpha)$ holds, so does $\Delta(\alpha')$ for any $\alpha' < \alpha$.

Now we turn to the proof of Proposition 5.2.

Proof of Proposition 5.2. The proof comes from Delmotte of [18].

The first assertion in Lemma 5.1 implies, for any $n \in \mathbb{N}$,

$$p_n(x, y) \le C(\beta)\mathcal{P}_n(x, y).$$

The upper bound, then, is an immediate consequence of Theorem 5.1: for any $x, y \in V$,

$$p_n(x, y) \le \frac{C(\beta)Cm(y)}{V(x, \sqrt{n})} = \frac{C_d m(y)}{V(x, \sqrt{n})}.$$

The second assertion is a little more complicated.

Suppose, for a minute, that for any $\varepsilon > 0$, there exists an $a > 0$ such that

$$\sum_{|k-(1-\alpha)n|>a\sqrt{n}} a_k \overline{p}_k(x, y) \le \frac{\varepsilon m(y)}{V(x, \sqrt{n})}. \tag{5.5}$$

We return briefly to prove that such an a always exists. Fix such an a for a sufficiently small ε, taking, say,

$$0 < \varepsilon < \frac{1}{2}C' \le \frac{1}{2}\mathcal{P}_n(x, y) \cdot \frac{V(x, \sqrt{n})}{m(y)}.$$

We set $\alpha = \frac{\beta}{2}$, and $n \ge N = \frac{a^2}{\alpha^2}$. For such choices, the second assertion of Lemma 5.1 implies that

$$\begin{aligned} p_n(x, y) &\ge \sum_{|k-(1-\alpha)n|\le a\sqrt{n}} b_k \overline{p}_k(x, y) \\ &\ge C(a, \alpha) \sum_{|k-(1-\alpha)n|\le a\sqrt{n}} a_k \overline{p}_k(x, y), \end{aligned}$$

and furthermore

$$\begin{aligned} C(a, \alpha)\mathcal{P}_n(x, y) &= C(a, \alpha) \sum_{|k-(1-\alpha)n|\le a\sqrt{n}} a_k \overline{p}_k(x, y) \\ &\quad + C(a, \alpha) \sum_{|k-(1-\alpha)n|>a\sqrt{n}} a_k \overline{p}_k(x, y) \\ &\le p_n(x, y) + C(a, \alpha) \sum_{|k-(1-\alpha)n|>a\sqrt{n}} a_k \overline{p}_k(x, y) \\ &\le p_n(x, y) + C(a, \alpha)\frac{\varepsilon m(y)}{V(x, \sqrt{n})}. \end{aligned}$$

Since we assume $n \ge d(x, y)^2$, by applying the second assertion of (5.4) we obtain

$$\begin{aligned} p_n(x, y) &\ge C(a, \alpha)\left(\mathcal{P}_n(x, y) - \frac{\varepsilon m(y)}{V(x, \sqrt{n})}\right) \\ &\ge C(a, \alpha)\left(\frac{C'm(y)}{V(x, \sqrt{n})} - \frac{\varepsilon m(y)}{V(x, \sqrt{n})}\right) \\ &= \frac{c_d m(y)}{V(x, \sqrt{n})}, \end{aligned}$$

as desired.

Thus it remains to prove that (5.5) can be satisfied. First consider another, slightly modified, Markov kernel $p' = \frac{\overline{p}}{1-\alpha}$. Such a kernel is generated by weights ω'_{xy} as follows:

$$\begin{aligned} \omega'_{xx} &= \frac{\omega_{xx} - \alpha m(x)}{1-\alpha} \geq \alpha m(x) \quad \text{for all } x \in V, \\ \omega'_{xy} &= \frac{\omega_{xy}}{1-\alpha} \qquad\qquad\qquad \text{for all } x \neq y \in V, \\ m'(x) &= m(x). \end{aligned}$$

Note that $\Delta(\alpha)$ is true in G with the new weights. Condition $\mathrm{CDE}'(n_0, 0)$ also still holds for the new weights, because if one lets Δ' be the new Laplacian for ω'_{xy}, then for any $f, g \in V^{\mathbb{R}}$ we obtain

$$\begin{aligned} \Delta' f(x) &= \frac{1}{1-\alpha}\Delta f(x), \qquad \Gamma'(f,g) = \frac{1}{1-\alpha}\Gamma(f,g), \\ \Gamma'_2(f,g) &= \frac{1}{(1-\alpha)^2}\Gamma_2(f,g), \quad \widetilde{\Gamma}'_2(f) = \frac{1}{(1-\alpha)^2}\widetilde{\Gamma}_2(f). \end{aligned}$$

Furthermore, the process of proving $\mathrm{DV}(C)$ still works when adding loops to every point of graph. Then $\mathrm{DV}(C)$ is still satisfied for the new weights. This yields

$$p'_k(x,y) \leq \frac{C'_d m(y)}{V(x,\sqrt{k})},$$

and hence

$$\overline{p}_k(x,y) \leq \frac{C'_d m(y)(1-\alpha)^k}{V(x,\sqrt{k})}.$$

Next, we prove the following estimate:

$$e^{(\alpha-1)n} \sum_{|k-(1-\alpha)n| > a\sqrt{n}} \frac{((1-\alpha)n)^k}{k!} \frac{1}{V(x,\sqrt{k})} \leq \frac{\varepsilon'}{V(x,\sqrt{n})}.$$

The sum for $k > a\sqrt{n} + (1-\alpha)n$ is easier because we simply use

$$V(x,\sqrt{k}) \geq V\left(x, \sqrt{\frac{n}{2}}\right) \geq V\left(x, \frac{\sqrt{n}}{2}\right) \geq \frac{V(x,\sqrt{n})}{C_1}$$

giving

$$\begin{aligned} &e^{(\alpha-1)n} \sum_{k > a\sqrt{n}+(1-\alpha)n} \frac{((1-\alpha)n)^k}{k!} \frac{1}{V(x,\sqrt{k})} \\ &\leq e^{(\alpha-1)n} \frac{C_1}{V(x,\sqrt{n})} \sum_{k > a\sqrt{n}+(1-\alpha)n} \frac{((1-\alpha)n)^k}{k!} \\ &\leq e^{(\alpha-1)n} \frac{C_1}{V(x,\sqrt{n})} \frac{((1-\alpha)n)^{(1-\alpha)n+a\sqrt{n}}}{(a\sqrt{n}+(1-\alpha)n)!} \frac{1}{1-\frac{(1-\alpha)n}{a\sqrt{n}+(1-\alpha)n}} \\ &\leq \frac{CC_1}{V(x,\sqrt{n})} \exp\left(a\sqrt{n} - (a\sqrt{n}+(1-\alpha)n)\log\left(1+\frac{a}{(1-\alpha)\sqrt{n}}\right)\right) \\ &\qquad \cdot \frac{1}{\sqrt{a\sqrt{n}+(1-\alpha)n}} \frac{a\sqrt{n}+(1-\alpha)n}{a\sqrt{n}} \\ &\leq \frac{\varepsilon'}{2V(x,\sqrt{n})} \end{aligned}$$

for our (arbitrary) choice of ε', so long as a is sufficiently large. The second to last inequality follows from the inequality

$$k! \geq \frac{k^k e^{-k}\sqrt{k}}{C}.$$

The final line holds by as our assumption $n \geq \frac{a^2}{\alpha^2}$ implies

$$\frac{1}{\sqrt{a\sqrt{n}+(1-\alpha)n}}\frac{a\sqrt{n}+(1-\alpha)n}{a\sqrt{n}} \leq \frac{1}{a}.$$

Finally, observe that, by the inequality

$$\log(1+u) \geq \frac{u}{1+u} + \frac{u^2}{2(1+u)^2}$$

for any real number $u \geq 0$, then the exponential is negative and for a sufficiently large a the claim holds.

Remark 3 allows us to deal with $1 \leq k < -a\sqrt{n}+(1-\alpha)n$. It gives

$$V(x,\sqrt{k}) \leq C\left(\frac{\sqrt{k}}{\sqrt{k-1}}\right)^{\frac{\log C}{\log 2}} V(x,\sqrt{k-1}) \leq C_2 V(x,\sqrt{k-1}).$$

The terms $1 \leq k \leq \frac{(1-a)n}{2C_2}$ satisfy

$$\frac{((1-\alpha)n)^{k-1}}{(k-1)!}\frac{1}{V(x,\sqrt{k-1})} \leq \frac{1}{2}\frac{((1-\alpha)n)^k}{k!}\frac{1}{V(x,\sqrt{k})},$$

and the estimate is straightforward. When $\frac{(1-a)n}{2C_2} < k < -a\sqrt{n}+(1-\alpha)n$, applying Remark 3 gives

$$V(x,\sqrt{k}) \geq V\left(x,\sqrt{\frac{(1-a)n}{2C_2}}\right) \geq C_3 V(x,\sqrt{n}).$$

This completes the proof. □

To prove our discrete-time Gaussian upper bounds, we first recall the following result from [14].

Theorem 5.3. *For a reversible nearest neighborhood random walk on the locally finite graph $G = (V, E)$, the following properties are equivalent:*

(1) *The relative Faber–Krahn inequality* (FK).

(2) *The discrete-time Gaussian upper estimate in conjunction with the doubling property* $\mathrm{DV}(C)$.

(3) *The discrete-time on-diagonal upper estimate in conjunction with the doubling property* $\mathrm{DV}(C)$.

Now we complete the proof of the discrete-time Gaussian estimate.

Theorem 5.4. *Suppose that G is a locally finite graph satisfying* $\mathrm{CDE}'(n_0, 0)$ *and* $\Delta(\alpha)$. *Then G satisfies the discrete-time Gaussian estimate* $\mathrm{G}(c_l, C_l, C_r, c_r)$.

Proof. We have already observed that the discrete-time on-diagonal upper estimate and the doubling property $\mathrm{DV}(C)$ both hold for graphs satisfying $\mathrm{CDE}'(n_0, 0)$ and $\Delta(\alpha)$. Theorem 5.3 immediately implies the discrete-time Gaussian upper estimate.

The lower bound follows from the on-diagonal one. The strategy is similar to Delmotte of [18]. We repeatedly apply the second assertion of Proposition 5.2. Set $n = n_1 + n_2 + \cdots + n_j$, $x = x_0, x_1, \ldots, x_j = y$ and $B_0 = x$, $B_i = B(x_i, r_i)$, $B_j = y$ such that

$$\begin{cases} j - 1 \leq C\frac{d(x,y)^2}{n}, & \\ r_i \geq c\sqrt{n_{i+1}}, & \text{so that } V(z, \sqrt{n_{i+1}}) \leq AV(B_i), \text{ when } z \in B_i, \\ \sup_{z \in B_{i-1}, z' \in B_i} d(z, z')^2 \leq n_i, & \text{so that } p_{n_i}(z, z') \geq \frac{c_d m(z')}{V(z, \sqrt{n_i})}. \end{cases}$$

Such a decomposition allows us to immediately derive the lower bound. Indeed,

$$\begin{aligned} p_n(x, y) &\geq \sum_{(z_1, \ldots, z_{j-1}) \in B_1 \times \cdots \times B_{j-1}} p_{n_1}(x, z_1) p_{n_2}(z_1, z_2) \cdots p_{n_j}(z_{j-1}, y) \\ &\geq \sum_{(z_1, \ldots, z_{j-1}) \in B_1 \times \cdots \times B_{j-1}} \frac{c_d m(z_1)}{V(x, \sqrt{n_1})} \frac{c_d m(z_2)}{V(z_1, \sqrt{n_2})} \cdots \frac{c_d m(y)}{V(z_{j-1}, \sqrt{n_j})} \\ &\geq c_d^j A^{1-j} \sum_{(z_1, \ldots, z_{j-1}) \in B_1 \times \cdots \times B_{j-1}} \frac{m(z_1)}{V(x, \sqrt{n_1})} \frac{m(z_2)}{V(B_1)} \cdots \frac{m(y)}{V(B_j)} \\ &= \frac{c_d m(y)}{V(x, \sqrt{n_1})} \left(\frac{c_d}{A}\right)^{j-1}. \end{aligned}$$

If we choose $C_l \geq C \log(\frac{A}{c_d})$, and $V(x, \sqrt{n_1}) \leq V(x, \sqrt{n})$, the Gaussian lower bound

$$p_n(x, y) \geq \frac{c_d m(y)}{V(x, \sqrt{n})} e^{-C_l \frac{d(x,y)^2}{n}},$$

and thus the theorem, follows. □

From the discrete-time Gaussian estimate, we return to derive a continuous-time Gaussian lower bound estimate for small t promised in the discussion after Theorem 5.1.

Remark 4. If G is a graph satisfying $\mathrm{CDE}'(n_0, 0)$, and $\Delta(\alpha)$ and t is sufficiently small, then for any $x, y \in V$,

$$\mathcal{P}_t(x, y) \geq \frac{C' m(y)}{V(x, \sqrt{t})} \exp\left(-c' \frac{d(x, y)^2}{t}\right)$$

holds, with c', C' depending on the dimension parameter n_0 and α.

Proof. We first consider $d(x, y) = 0$; in other words when $x = y$. We need to prove that

$$\mathcal{P}_t(x, x) \geq \frac{C' m(x)}{V(x, \sqrt{t})}$$

when t for small t. In fact, the relationship between the continuous-time heat kernel and the discrete-time heat kernel (5.1) gives that for any $t > 0$,

$$\begin{aligned}\mathcal{P}_t(x,x) &= e^{-t}\sum_{k=0}^{+\infty}\frac{t^k}{k!}p_k(x,x)\\ &= e^{-t}p_0(x,x) + e^{-t}\sum_{k\geq 1}\frac{t^k}{k!}p_k(x,y)\\ &\geq e^{-t}p_0(x,x) = e^{-t}.\end{aligned}$$

For sufficiently small t, then, $\mathcal{P}_t(x,x) \geq C'$ for some $C' > 0$. On the other hand, one has $V(x,\sqrt{t}) = m(x)$ when t is small enough and so the desired lower bound holds.

Now we consider $d(x,y) \geq 1$. When $k < d(x,y)$, clearly $p_k(x,y) = 0$. We obtain

$$\begin{aligned}\mathcal{P}_t(x,y) &= e^{-t}\sum_{k=0}^{+\infty}\frac{t^k}{k!}p_k(x,y)\\ &= e^{-t}\sum_{k\geq d(x,y)}\frac{t^k}{k!}p_k(x,y)\\ &\geq e^{-t}\sum_{k\geq d(x,y)}\frac{t^k}{k!}\frac{c_d m(y)}{V(x,\sqrt{k})}e^{-C_l\frac{d(x,y)^2}{k}}\\ &\geq e^{-t}\frac{t^{(d(x,y)+1)}}{(d(x,y)+1)!}\frac{c_d m(y)}{V(x,\sqrt{d(x,y)+1})}e^{-C_l\frac{d(x,y)^2}{d(x,y)+1}}\\ &\quad + e^{-t}\sum_{k\neq d(x,y)+1,\,k\geq d(x,y)}\frac{t^k}{k!}\frac{c_d m(y)}{V(x,\sqrt{k})}e^{-C_l\frac{d(x,y)^2}{k}}\\ &\geq e^{-t}\frac{t^{(d(x,y)+1)}}{(d(x,y)+1)!}\frac{c_d m(y)}{V(x,\sqrt{d(x,y)+1})}e^{-C_l(d(x,y)+1)}\\ &\geq \frac{c_d e^{-t}}{C_0}\frac{m(y)}{m(x)}\cdot\frac{e^{-C_l(d(x,y)+1)}t^{(d(x,y)+1)}}{(d(x,y)+1)^{n_0}(d(x,y)+1)!}.\end{aligned}$$

In the third step, we apply the discrete-time Gaussian lower bound estimate of heat kernel $p_k(x,y)$ under the assumption of CDE$'(n_0,0)$ and $\Delta(\alpha)$ from Theorem 5.4. In the fourth step, we separate the sum in to two parts to emphasize that, in the fifth step, we drop the (positive) second part and keep only the term $k = d(x,y)+1 > 1$ from the original summation. Finally, we use polynomial volume growth in the last step (which follows from condition CDE$(n_0,0)$ and hence from CDE$'(n_0,0)$) from [8, Corollary 7.8]. This states that, under CDE$(n_0,0)$, there exists a constant $C_0 > 0$ such that, for any $r > 1$,

$$V(x,\sqrt{r}) \leq C_0 m(x) r^{n_0}.$$

To finish, consider the following function f, where here $d = d(x,y) \geq 1$:

$$\begin{aligned}f(t,d) &= -\frac{t}{d^2}\ln\left(\frac{e^{-C_l(d+1)}t^{(d+1)}}{(d+1)^{n_0}(d+1)!}\right)\\ &= -t\ln t\,\frac{d+1}{d^2} + t\left(\frac{C_l(d+1)}{d^2} + n_0\frac{\ln(d+1)}{d^2} + \frac{\ln(d+1)!}{d^2}\right) \to 0 \quad (t\to 0^+),\end{aligned}$$

One easily observes that $f(t,d)$ is positive for t small enough, and moreover both $\frac{d+1}{d^2}$ and $\frac{C_l(d+1)}{d^2} + n_0\frac{\ln(d+1)}{d^2} + \frac{\ln(d+1)!}{d^2}$ are bounded by a constant not depending on d. Thus, for t small enough, there exists a constant $c' > 0$ independent of d such that

$$f(t,d) \leq c'.$$

But then, for all positive integers $d \geq 1$,

$$\frac{e^{-C_l(d+1)}t^{(d+1)}}{(d+1)^{n_0}(d+1)!} \geq \exp\left(-c'\frac{d^2}{t}\right) \quad (t \to 0^+).$$

Moreover, when t is small enough, $V(x,\sqrt{t}) = m(x)$, and e^{-t} is bounded. Combining, we obtain

$$\mathcal{P}_t(x,y) \geq \frac{C'm(y)}{V(x,\sqrt{t})}\exp\left(-c'\frac{d(x,y)^2}{t}\right) \quad (t \to 0^+).$$

This completes the proof. □

Combining yields the following.

Theorem 5.5. *Suppose that G is a locally finite graph satisfying* $\mathrm{CDE}'(n_0,0)$ *and* $\Delta(\alpha)$. *Then G satisfies the following four properties:*

(1) *There exist $C_1, C_2, \alpha > 0$ such that* $\mathrm{DV}(C_1)$, $\mathrm{P}(C_2)$, *and* $\Delta(\alpha)$ *are true.*

(2) *There exist $c_l, C_l, C_r, c_r > 0$ such that* $\mathrm{G}(c_l, C_l, C_r, c_r)$ *is true.*

(3) *For any $\eta \in (0,1)$ and $0 < \theta_1 < \theta_2 < \theta_3 < \theta_4$, there exists a constant C_H such that* $\mathrm{H}(\eta,\theta_1,\theta_2,\theta_3,\theta_4,C_H)$ *is true.*

(3)' *For any $\eta \in (0,1)$ and $0 < \theta_1 < \theta_2 < \theta_3 < \theta_4$, there exists a constant $C_{\mathcal{H}}$ such that* $\mathcal{H}(\eta,\theta_1,\theta_2,\theta_3,\theta_4,C_{\mathcal{H}})$ *is true.*

Proof. Condition $\mathrm{CDE}'(n_0,0)$ implies $\mathrm{DV}(C_1)$ (by Theorem 4.2), and Theorem 5.4 states that $\mathrm{CDE}'(n_0,0)$ and $\Delta(\alpha)$ implies $\mathrm{G}(c_l, C_l, C_r, c_r)$. From (2), work of Delmotte in [18] implies that $\mathrm{P}(C_2)$ is true, and that (3) and (3)' hold as well. □

6. Diameter bounds

In this section we will show another application of Theorem 3.2. We prove that positively curved graphs (that is, graphs satisfying $\mathrm{CDE}'(n,K)$ for some $K > 0$ are finite. In order to prove this, we consider an alternate to the graph distance function on a graph, the so-called canonical distance and diameter of G associated with a Laplace operator Δ:

$$\widetilde{d}(x,y) = \sup_{f\in\ell^\infty(V,\mu),\, \|\Gamma(f)\|_\infty \leq 1} |f(x)-f(y)|, \quad x,y \in V,$$
$$\widetilde{D} = \sup_{x,y\in V} \widetilde{d}(x,y).$$

This distance was introduced in [9], and has been used for example in [1,25,29]. In this section we are concerned with simple, connected and loopless graphs.

6.1. Global heat kernel bounds. In this subsection, under the assumption that a graph is positively curved, we prove a bound on the total measure of a graph. This is used to derive a global heat kernel bound, and ultimately to establish that the graph's diameter is finite. The most crucial of these steps is an estimate proving that the total measure of the graph is finite.

We apply Theorem 3.2, choosing γ in a such a way that

$$\alpha' - \frac{4\alpha\gamma}{n} + 2\alpha K = 0.$$

That is, choose

$$\gamma = \frac{n}{4}\left(\frac{\alpha'}{\alpha} + 2K\right).$$

Integrating both sides of the inequality (3.3) from 0 to T, we obtain

$$\begin{aligned}\alpha(T)\frac{P_T(\Gamma(\sqrt{f}))}{P_T f} &- \alpha(0)\frac{\Gamma(\sqrt{P_T f})}{P_T f} \\ &\geq \frac{2}{n}\left(\int_0^T \alpha\gamma\, dt\right)\frac{\Delta P_T(f)}{P_T f} - \frac{2}{n}\int_0^T \alpha\gamma^2\, dt.\end{aligned} \tag{6.1}$$

Our first result in the subsection is the following.

Proposition 6.1. *Let $G = (V, E)$ be a locally finite, connected graph satisfying condition* $\mathrm{CDE}'(n, K)$ *for some $K > 0$. Then, for all $0 < \theta < K$ and $t_0 > 0$, there exists a constant $C_1 > 0$ such that for every non-negative f satisfying $\|f\|_\infty \leq 1$, and every $t \geq t_0$,*

$$|\sqrt{P_t f}(x) - \sqrt{P_t f}(y)| \leq C_1 e^{-\frac{\theta}{2}t}\widetilde{d}(x, y), \quad x, y \in V.$$

Remark. Of course, it is easy to replace the assumption that $\|f\|_\infty \leq 1$ by $\|f\|_\infty \leq M$ for any $M \geq 0$.

Proof. Fix some $0 < \theta < K$ and some $0 < t_0 \leq T$. We show the inequality holds at time T assuming T is sufficiently large. In (6.1), we take

$$\alpha(t) = 2Ke^{-\theta t}(e^{-\theta t} - e^{-\theta T})^{\frac{2K}{\theta}-1},$$

so that

$$\alpha(0) = 2K(1 - e^{-\theta T})^{\frac{2K}{\theta}-1} \quad \text{and} \quad \alpha(T) = 0.$$

With such a choice a simple computation gives

$$\gamma = \frac{n}{4}\left(-e^{-\theta T}\frac{2K - \theta}{e^{-\theta t} - e^{-\theta T}}\right),$$

which is non-positive for $0 \leq t \leq T$. Then, for any $T > 0$,

$$-Kn(1 - e^{-\theta T})^{\frac{2K}{\theta}-1}\frac{\Gamma(\sqrt{P_T f})}{P_T f} \geq \left(\int_0^T \alpha\gamma\, dt\right)\frac{\Delta P_T(f)}{P_T f} - \int_0^T \alpha\gamma^2\, dt. \tag{6.2}$$

Now, we compute

$$\int_0^T \alpha\gamma\, dt = -\frac{nK}{2}(1 - e^{-\theta T})^{\frac{2K}{\theta}-1}(e^{-\theta T})$$

and

$$\int_0^T a\gamma^2\, dt = \frac{Kn^2}{8}(1 - e^{-\theta T})^{\frac{2K}{\theta}-2}e^{-2\theta T} \times \left(\frac{\theta(\frac{2K}{\theta} - 1)^2}{\frac{2K}{\theta} - 2}\right).$$

We thus obtain from (6.2) that for any $T > t_0 \geq 0$,

$$
\begin{aligned}
(6.3) \qquad 0 &\geq -Kn(1-e^{-\theta T})^{\frac{2K}{\theta}-1}\frac{\Gamma(\sqrt{P_T f})}{P_T f} \\
&\geq -\frac{nK}{2}(1-e^{-\theta T})^{\frac{2K}{\theta}-1}e^{-\theta T}\frac{\Delta P_T f}{P_T f} \\
&\quad - \frac{Kn^2\theta(\frac{2K}{\theta}-1)^2}{8(\frac{2K}{\theta}-2)}(1-e^{-\theta T})^{\frac{2K}{\theta}-2}e^{-2\theta T}.
\end{aligned}
$$

Dividing, and switching notation from T to t, we obtain that

$$
(6.4) \qquad \Gamma(\sqrt{P_t f}) \leq \frac{1}{2}e^{-\theta t}\Delta P_t f + \frac{n\theta(\frac{2K}{\theta}-1)^2}{4(\frac{2K}{\theta}-2)(1-e^{-\theta t})}e^{-2\theta t}P_t f \leq C_1^2 e^{-\theta t},
$$

with

$$
C_1 = \sqrt{D_\mu + \frac{n\theta(\frac{2K}{\theta}-1)^2}{8(\frac{2K}{\theta}-2)(e^{\theta t_0}-1)}}.
$$

Consider the function

$$
u(x) = \frac{1}{C_1}e^{\frac{\theta}{2}t}\sqrt{P_t f}(x) \in \ell^\infty(V,\mu).
$$

By construction, we have normalized u so that for any $t \geq t_0$, $\|\Gamma(u)\|_\infty \leq 1$. By the definition of the canonical distance $\widetilde{d}(x,y)$,

$$
|u(x)-u(y)| \leq \widetilde{d}(x,y),
$$

In turn,

$$
|\sqrt{P_t f}(x) - \sqrt{P_t f}(y)| \leq C_1 e^{-\frac{\theta}{2}t}\widetilde{d}(x,y).
$$

as desired. □

Proposition 6.2. *Let $G = (V,E)$ be a locally finite, connected graph satisfying condition* $\mathrm{CDE}'(n,K)$ *for some $K > 0$. Then, for all $0 < \theta < K$ and $t_0 > 0$, there exists a constant $C_2 > 0$ such that for every non-negative function f with $\|f\|_\infty \leq 1$, and for every $t \geq t_0$,*

$$
|\partial_t P_t f| \leq C_2 e^{-\frac{\theta}{2}t}.
$$

Proof. Let $P_t f = u$. Then

$$
\begin{aligned}
|\Delta u| &\leq \widetilde{\sum_{y\sim x}}|u(y)-u(x)| \\
&= \widetilde{\sum_{y\sim x}}(\sqrt{u}(y)+\sqrt{u}(x))|\sqrt{u}(y)-\sqrt{u}(x)| \\
&\leq \left(\widetilde{\sum_{y\sim x}}(\sqrt{u(y)}+\sqrt{u(x)})^2\right)^{\frac{1}{2}}\left(\widetilde{\sum_{y\sim x}}(\sqrt{u(y)}-\sqrt{u(x)})^2\right)^{\frac{1}{2}} \\
&\leq 2\sqrt{2D_\mu}C\sqrt{\Gamma(\sqrt{u})}.
\end{aligned}
$$

Combing with (6.4), we let $C_2 = 2\sqrt{2D_\mu}\cdot C_1$. This yields the desired result. □

Proposition 6.3. *Let $G = (V, E)$ be a locally finite, connected graph satisfying condition* $\mathrm{CDE}'(n, K)$ *with $K > 0$. Then the measure μ is finite, that is, $\mu(V) < \infty$.*

Proof. By Proposition 6.2, the limit of $p(t, x, \cdot)$ exists and is finite when $t \to \infty$. Moreover, Proposition 6.1 along with property (2) of the heat kernel from Remark 2, imply that $\lim_{t\to\infty} p(t, x, \cdot)$ is some non-negative value $c(x) \geq 0$. The symmetry of the heat kernel implies that $c(x)$ actually does not depend on x.

To show the finiteness of the measure, it will suffice to prove that this limit is actually strictly positive under our assumption that $\mathrm{CDE}'(n, K)$ holds for some $K > 0$.

We apply the lower bound in Proposition 6.2, integrating it from some $t_1 > t_0$ to ∞ to obtain

$$\lim_{t\to\infty} p(t, x, \cdot) - p(t_1, x, y) = \int_{t_1}^{\infty} \partial_t p(t, x, \cdot)\, dt \geq -\frac{2C_2}{s} e^{-\frac{\theta}{2}t_1}.$$

Let $y = x$. Theorem 7 of [8] states that there is some constant $C' > 0$ so that

$$p(t_1, x, x) \geq \frac{C'}{t_1^n}$$

under condition $\mathrm{CDE}(n, 0)$, and hence $\mathrm{CDE}(n, K)$ – and hence $\mathrm{CDE}'(n, K)$ – for any $K > 0$. Thus combining,

$$\lim_{t\to\infty} p(t, x, x) \geq \frac{C'}{t_1^n} - \frac{2C_2}{\theta} e^{-\frac{\theta}{2}t_1} > 0.$$

This implies that $\lim_{t\to\infty} p(t, x, y) = c > 0$ for any $x, y \in V$. This, in turn, (from property (3) in Remark 2) implies that the measure μ is finite. □

Finally, we state a result from [22], which says the having infinite measure and having infinite diameter are equivalent properties for locally compact separable metric spaces M satisfying volume doubling (DV).

Lemma 6.1. *Assume that (M, d) is connected and satisfies* DV. *Then*

$$\mu(M) = \infty \iff \mathrm{diam}(M) = \infty.$$

Locally finite graphs satisfy the hypothesis of this lemma where d is the graph distance on graphs. We have already shown in Theorem 4.2 that a graph satisfying $\mathrm{CDE}'(n, 0)$ (and hence $\mathrm{CDE}'(n, K)$, as $\mathrm{CDE}'(n, K) \Rightarrow \mathrm{CDE}'(n, 0)$, for any $K > 0$) has the volume doubling property. Combining with Proposition 6.3 and the first equivalence in Lemma 6.1, we get the following statement that positively curved graphs have finite diameter.

Theorem 6.4. *Suppose that G is a locally finite, connected, simple graph satisfying condition* $\mathrm{CDE}'(n, K)$ *with $K > 0$. Then the diameter of G, in terms of the graph distance, is finite.*

Per Proposition 6.3, we may assume μ is a probability measure – renormalizing so that $\lim_{t\to\infty} p(t, x, \cdot) = 1$.

Proposition 6.5. *Suppose that G is a connected, locally finite graph satisfying condition* $\mathrm{CDE}'(n, K)$ *with $K > 0$. Then, for any $x, y \in V$, $t > 0$,*

$$p(t, x, y) \leq \frac{1}{(1 - e^{-\frac{2K}{3}t})^n}.$$

Proof. We apply (6.3) with $\theta = \frac{2K}{3}$. Considering $p(\tau, x, y)$, we obtain

$$\partial_\tau \log p(\tau, x, y) \geq -\frac{2nK}{3} \frac{e^{-\theta\tau}}{1 - e^{-\theta\tau}}.$$

Integrating from t to ∞, and using the fact that $\lim_{t\to\infty} p(t, x, y) = 1$ gives

$$p(t, x, y) \leq \frac{1}{(1 - e^{-\theta t})^n}.$$

This ends the proof. □

6.2. Diameter bounds. In this subsection we derive an explicit diameter bound for graphs satisfying $\mathrm{CDE}'(n, K)$.

The idea is to prove that the operator Δ satisfies an entropy-energy inequality, as mentioned in the introduction. First we derive, for graphs, an analogue of Davies' theorem ([15]) on manifolds. Note that, obviously, if μ is a finite measure, $f \in \ell^\infty(V, \mu)$ implies $f \in \ell^p(V, \mu)$ for any $p > 1$.

Lemma 6.2. *Suppose that G is a locally finite, connected graph with $\mu(V)$ bounded. Let $f \in \ell^\infty(V, \mu)$ satisfy $\|P_t f\|_\infty \leq e^{M(t)} \|f\|_2$ for some continuous and decreasing function $M(t)$. If $\|f\|_2 = 1$, then for any $t > 0$,*

$$\sum_{x\in V} \mu(x) f^2(x) \ln f^2(x) \leq 2t \sum_{x\in V} \mu(x)\Gamma(f)(x) + 2M(t).$$

Proof. Let $p(s)$ be a bounded, continuous function with $p(s) \geq 1$ and $p'(s)$ bounded. For any function $0 \leq f \in \ell^\infty(V, \mu)$, consider the function $(P_s f)^{p(s)}$. Note that $(P_s f)^{p(s)}$ is in $\ell^1(V, \mu)$. Likewise, the two functions $(P_s f)^{p(s)} \ln P_s f$ and $\Delta P_s f (P_s f)^{p(s)-1}$ are also in $\ell^1(V, \mu)$. (Note here that at $s = 0$, if $f = 0$, we take $(P_s f)^{p(s)} \ln P_s f$ to be zero as well.) This tells us that

$$\begin{aligned}
\frac{d}{ds}\|P_s f\|_{p(s)}^{p(s)} &= \frac{d}{ds} \sum_{x\in V} \mu(x)(P_s f(x))^{p(s)} \\
&= \sum_{x\in V} \mu(x) \frac{d}{ds}(P_s f(x))^{p(s)} \\
&= \sum_{x\in V} \mu(x)\big(p'(s)(P_s f(x))^{p(s)} \ln P_s f(x) + p(s)(P_s f(x))'(P_s f(x))^{p(s)-1}\big) \\
&= p'(s) \sum_{x\in V} \mu(x)(P_s f(x))^{p(s)} \ln P_s f(x) \\
&\quad + p(s) \sum_{x\in V} \mu(x)\Delta P_s f(x)(P_s f(x))^{p(s)-1}.
\end{aligned}$$

At $s = 0$, specializing to $p(s) = \frac{2t}{t-s}$ (where $0 \le s \le t - t_1$, with $t > t_1 > 0$) gives

$$\frac{d}{ds}\|P_s f\|_{p(s)}^{p(s)}\Big|_{s=0} = \frac{2}{t}\sum_{x\in V}\mu(x)f^2(x)\ln f(x) + 2\sum_{x\in V}\mu(x)f(x)\Delta f(x).$$

On the other hand, we give a lower bound on this derivative. Combining our assumption that $\|P_t f\|_\infty \le e^{M(t)}\|f\|_2$, for continuous and decreasing $M(t)$ and our assumption that $\|f\|_2 = 1$, and using the Stein interpolation theorem, we obtain

$$\|P_s f\|_{p(s)} \le e^{\frac{M(t)s}{t}}.$$

Then

$$\frac{d}{ds}\|P_s f\|_{p(s)}^{p(s)}\Big|_{s=0} \le \frac{2M(t)}{t}.$$

This holds due to the fact that

$$\|P_s f\|_{p(s)}^{p(s)}\Big|_{s=0} = \|p(s)\|_2 = 1,$$

and $e^{\frac{M(t)sp(s)}{t}}|_{s=0} = 1$. Direct computation gives

$$1 \ge \lim_{s\to 0^+}\frac{\|P_s f\|_{p(s)}^{p(s)} - 1}{e^{\frac{M(t)sp(s)}{t}} - 1} = \frac{d}{ds}\|P_s f\|_{p(s)}^{p(s)}\Big|_{s=0}\frac{t}{2M(t)}.$$

The identity

$$-\sum_{x\in V}\mu(x)f(x)\Delta f(x) = \sum_{x\in V}\mu(x)\Gamma(f)(x)$$

holds for any $f \in \ell^\infty(V,\mu)$. Combining with the above equality gives

$$\sum_{x\in V}\mu(x)f^2(x)\ln f^2(x) \le 2t\sum_{x\in V}\mu(x)\Gamma(f)(x) + 2M(t), \quad t > t_1.$$

This completes the proof. □

Proposition 6.6. *Let $G = (V, E)$ be a locally finite, connected graph satisfying condition* $\mathrm{CDE}'(n, K)$. *Any $0 \le f \in \ell^\infty(V,\mu)$ such that $\|f\|_2 = 1$ satisfies*

$$\sum_{x\in V}\mu(x)f^2(x)\ln f^2(x) \le \Phi\Big(\sum_{x\in V}\mu(x)\Gamma(f)(x)\Big),$$

where

$$\Phi(x) = 2n\Big[\Big(1 + \frac{1}{\theta n}x\Big)\ln\Big(1 + \frac{1}{\theta n}x\Big) - \frac{1}{\theta n}x\ln\Big(\frac{1}{\theta n}x\Big)\Big].$$

Proof. Fix such an f. Using Proposition 6.5 and the Cauchy–Schwarz inequality gives

$$\|P_t f\|_\infty \le \frac{1}{(1 - e^{-\theta t})^n}\|f\|_2,$$

where $\theta = \frac{2K}{3}$. Therefore from Lemma 6.2, we obtain

$$\sum_{x\in V}\mu(x)f^2(x)\ln f^2(x) \le 2t\sum_{x\in V}\mu(x)\Gamma(f)(x) - 2n\ln(1 - e^{-\theta t}), \quad t > t_1 > 0.$$

By minimizing the right-hand side of the above inequality over t, we obtain

$$\begin{aligned}\sum_{y\in V}\mu(y)f^2(y)\ln f^2(y) &\le -\frac{2}{\theta}x\ln\Big(\frac{x}{x+\theta n}\Big)+2n\ln\Big(\frac{x+\theta n}{\theta n}\Big)\\ &= 2n\Big[\Big(1+\frac{1}{\theta n}x\Big)\ln\Big(1+\frac{1}{\theta n}x\Big)-\frac{1}{\theta n}x\ln\Big(\frac{1}{\theta n}x\Big)\Big],\end{aligned}$$

where $x=\sum_{y\in V}\mu(y)\Gamma(f)(y)$. □

We observe that Φ is a non-negative, monotonically increasing, and concave function, as we shall use these properties later.

In order to finish the result and bound the diameter, we first define some notation. For a positive bounded real-valued function f on V, let $E(f)$ denote the entropy of f with respect to μ defined by

$$E(f)=\sum_{x\in V}\mu(x)f(x)\ln f(x)-\sum_{x\in V}\mu(x)f(x)\ln\Big(\sum_{x\in V}\mu(x)f(x)\Big).$$

To ease the notation, we use

$$\int f\,d\mu=\sum_{x\in V}\mu(x)f(x).$$

The Laplace operator Δ satisfies a *logarithmic Sobolev inequality* if there exists a $\rho>0$ such that for all functions $f\in\ell^\infty(V,\mu)$,

$$\rho E(f^2)\le 2\int\Gamma(f)\,d\mu,$$

Equivalently, it suffices to say that a general logarithmic Sobolev inequality holds if all $f\in\ell^\infty(V,\mu)$ with $\|f\|_2=1$ satisfy

$$E(f^2)\le\Phi\Big(\int\Gamma(f)\,d\mu\Big), \tag{6.5}$$

where Φ is a concave and non-negative function on $[0,\infty)$.

Proposition 6.7. *Suppose that Δ satisfies a general logarithmic Sobolev inequality, and the function Φ from* (6.5) *is non-negative and monotonically increasing. Then G has diameter*

$$\widetilde{D}\le\sqrt{2}\int_0^\infty\frac{1}{x^2}\Phi(x^2)\,dx.$$

Proof. Consider any function $g\in\ell^\infty(V,\mu)$, with $\|\Gamma(g)\|_\infty\le 1$. Let $f_\lambda=e^{\lambda g}$ for some $\lambda\in\mathbb{R}^+$. We will apply (6.5) to the family of non-negative functions

$$\widetilde{f_\lambda}=\frac{f_{\lambda/2}}{\|f_{\lambda/2}\|_2}.$$

Let

$$G(\lambda)=\|f_{\lambda/2}\|_2^2=\int e^{\lambda g}\,d\mu$$

and observe that

$$G'(\lambda)=\int ge^{\lambda g}\,d\mu\ \Big(=\frac{1}{\lambda}\int f_{\lambda/2}^2\ln f_{\lambda/2}^2\,d\mu\Big).$$

On one hand, it is immediate by the definition of $\widetilde{f}$ that

$$E(\widetilde{f}_\lambda^2) = \frac{1}{G(\lambda)}\big(\lambda G'(\lambda) - G(\lambda)\ln G(\lambda)\big).$$

We also must consider the right-hand side of the Sobolev inequality, which contains a term of the form

$$\int \Gamma(\widetilde{f}_\lambda)\,d\mu = \frac{1}{\|f_{\lambda/2}\|_2^2}\int \Gamma(e^{\frac{\lambda g}{2}})\,d\mu.$$

Such terms can be bounded as follows:

$$\begin{aligned}
\int \Gamma(e^{\frac{\lambda g}{2}})\,d\mu &= \frac{1}{2}\sum_{x\in V}\sum_{y\sim x}\omega_{xy}\Big(e^{\frac{\lambda g(y)}{2}} - e^{\frac{\lambda g(x)}{2}}\Big)^2 \\
&= \frac{1}{2}\sum_{x\in V}\sum_{\substack{y\sim x\\ g(x)>g(y)}}\omega_{xy}\Big(e^{\frac{\lambda g(y)}{2}} - e^{\frac{\lambda g(x)}{2}}\Big)^2 \\
&\qquad + \frac{1}{2}\sum_{x\in V}\sum_{\substack{y\sim x\\ g(x)<g(y)}}\omega_{xy}\Big(e^{\frac{\lambda g(y)}{2}} - e^{\frac{\lambda g(x)}{2}}\Big)^2 \\
&= \sum_{x\in V}\sum_{\substack{y\sim x\\ g(x)>g(y)}}\omega_{xy}\Big(e^{\frac{\lambda g(y)}{2}} - e^{\frac{\lambda g(x)}{2}}\Big)^2 \\
&\le \sum_{x\in V}\sum_{\substack{y\sim x\\ g(x)>g(y)}}\omega_{xy}\Big(e^{\frac{\lambda}{2}(g(y)-g(x))} - 1\Big)^2 e^{\lambda g(x)} \\
&\le \frac{\lambda^2}{4}\sum_{x\in V}e^{\lambda g(x)}\sum_{\substack{y\sim x\\ g(x)>g(y)}}\omega_{xy}(g(y)-g(x))^2 \\
&\le \frac{\lambda^2}{2}\int e^{\lambda g}\Gamma(g)\,d\mu.
\end{aligned}$$

Since $\Gamma(g) \le 1$, and the function Φ is monotonically increasing, one has

$$\Phi\Big(\int \Gamma(\widetilde{f_\lambda})\,d\mu\Big) = \Phi\Big(\frac{1}{\|f_{\lambda/2}\|_2^2}\int \Gamma(e^{\frac{\lambda g}{2}})\,d\mu\Big) \le \Phi\Big(\frac{\lambda^2}{2}\Big).$$

By the logarithmic Sobolev inequality,

$$\lambda G'(\lambda) - G(\lambda)\ln G(\lambda) \le G(\lambda)\Phi\Big(\frac{\lambda^2}{2}\Big).$$

Let $H(\lambda) = \frac{1}{\lambda}\ln G(\lambda)$. Then the above inequality reads

$$H'(\lambda) \le \frac{1}{\lambda^2}\Phi\Big(\frac{\lambda^2}{2}\Big).$$

Since $H(0) = \lim_{\lambda\to 0}\frac{1}{\lambda}\ln G(\lambda) = \int g\,d\mu$, it follows that

$$H(\lambda) = H(0) + \int_0^\lambda H'(u)\,du \le \int g\,d\mu + \int_0^\lambda \frac{1}{u^2}\Phi\Big(\frac{u^2}{2}\Big)\,du.$$

Therefore for any $\lambda \geq 0$,

$$\sum_{x\in V} \mu(x) e^{\lambda(g(x) - \int g\, d\mu)} \leq \exp\left\{\lambda \int_0^\lambda \frac{1}{u^2} \Phi\left(\frac{u^2}{2}\right) du\right\}.$$

Let

$$C = \int_0^\infty \frac{1}{u^2} \Phi\left(\frac{u^2}{2}\right) du = \frac{1}{\sqrt{2}} \int_0^\infty \frac{1}{x^2} \Phi(x^2)\, dx.$$

Then, for every $\lambda \geq 0$ and $\varepsilon > 0$, when we apply the above inequality to g and $-g$ and apply Chebyshev's inequality,

$$\begin{aligned}
&\mu\left(\left\{x \in V : \left|g(x) - \int g\, d\mu\right| \geq C + \varepsilon\right\}\right) \\
&\quad \leq \sum_{\substack{x\in V \\ g(x) \geq \int g\, d\mu + C + \varepsilon}} \mu(x) + \sum_{\substack{x\in V \\ g(x) \leq \int g\, d\mu - C - \varepsilon}} \mu(x) \\
&\quad \leq \sum_{\substack{x\in V \\ g(x) \geq \int g\, d\mu + C + \varepsilon}} \frac{e^{\lambda(g(x) - \int g\, d\mu)}}{e^{\lambda(C+\varepsilon)}} \mu(x) + \sum_{\substack{x\in V \\ g(x) \leq \int g\, d\mu - C - \varepsilon}} \frac{e^{\lambda(-g(x) + \int g\, d\mu)}}{e^{\lambda(C+\varepsilon)}} \mu(x) \\
&\quad \leq 2e^{-\lambda(C+\varepsilon)} e^{\lambda C} \\
&\quad = 2e^{-\lambda\varepsilon} \to 0 \quad (\lambda \to \infty).
\end{aligned}$$

That is, we obtain

$$\left\| g(x) - \int g\, d\mu \right\|_\infty \leq C.$$

The diameter bound follow immediately by the definition of $\widetilde{D}$: Since g was arbitrary, one has

$$\widetilde{D} \leq \sqrt{2} \int_0^\infty \frac{1}{x^2} \Phi(x^2)\, dx,$$

as promised. □

Finally, we obtain:

Theorem 6.8. *Let G be a locally finite, connected graph satisfying* $\mathrm{CDE}'(n, K)$*, and* $K > 0$. *Then the diameter $\widetilde{D}$ of graph G in terms of canonical distance is finite, and*

$$\widetilde{D} \leq 4\sqrt{3}\pi \sqrt{\frac{n}{K}}.$$

Proof. Combining Proposition 6.6 and Proposition 6.7, we conclude that graphs satisfying $\mathrm{CDE}'(n, K)$ for some $K > 0$ also satisfy

$$\widetilde{D} \leq \sqrt{2} \int_0^\infty \frac{1}{x^2} \Phi(x^2)\, dx,$$

where

$$\Phi(x) = 2n\left[\left(1 + \frac{1}{\theta n} x\right) \ln\left(1 + \frac{1}{\theta n} x\right) - \frac{1}{\theta n} x \ln\left(\frac{1}{\theta n} x\right)\right],$$

and $\theta = \frac{2K}{3}$. Since

$$\begin{aligned}\int_0^\infty \frac{1}{x^2}\Phi(x^2)\,dx &= \frac{1}{2}\int_0^\infty \frac{1}{x^{\frac{3}{2}}}\Phi(x)\,dx \\ &= \int_0^\infty \frac{1}{\sqrt{x}}\Phi'(x)\,dx \\ &= -2\int_0^\infty \sqrt{x}\Phi''(x)\,dx < \infty,\end{aligned}$$

the diameter is finite, and $\Phi''(x) = -\frac{2n}{x(x+\theta n)}$. From this

$$-2\int_0^\infty \sqrt{x}\Phi''(x)\,dx = 4\pi\sqrt{\frac{n}{\theta}},$$

completing the proof. □

While this bounds the canonical diameter, it is possible to recover a bound for the usual graph distance. To this end, we first define intrinsic metrics. These give us a way to relate graph distance and canonical distance.

Intrinsic metrics on graphs were first introduced by Frank, Lenz and Wingert in [20]. A function $\rho : V \times V \to \mathbb{R}^+$ is called an intrinsic metric if, at all $x \in V$,

$$\sum_{y\sim x} \omega_{xy}\rho^2(x,y) \le \mu(x).$$

This induces a metric ρ on a graph via finding shortest paths. One example of such a function, given by Xueping Huang in his thesis [25], is the function, defined for all $x \in V$ and $y \sim x$,

$$\widetilde{\rho}(x,y) = \min\left\{\sqrt{\frac{\mu(x)}{m(x)}}, \sqrt{\frac{\mu(y)}{m(y)}}\right\},$$

where $m(x) = \sum_{y\sim x}\omega_{xy}$.

As mentioned, these metrics give a way of comparing graph distance with the canonical distance we have been using. Indeed, part (a) of the remark following [28, Definition 1.2] gives:

Proposition 6.9. *For any $x, y \in V$, the inequality following holds:*

$$\sqrt{2}\widetilde{\rho}(x,y) \le \widetilde{d}(x,y).$$

In fact, [28] shows that the above inequality holds for *any* intrinsic metric. For the metric $\tilde{\rho}$ in particular, under the assumption that D_μ is finite, then

$$\widetilde{\rho}(x,y) \ge \frac{d(x,y)}{\sqrt{D_\mu}}$$

for any x and y (by, again, extending the metric $\tilde{\rho}$ along shortest paths.)

The above inequalities, combined with Theorem 6.8 and Proposition 6.9, yield:

Theorem 6.10. *Suppose that G is a locally finite, connected graph and satisfies condition* $\mathrm{CDE}'(n,K)$ *with $K > 0$. Then the diameter, in terms of graph distance is finite, with a quantitative upper bound given by*

$$D \le 2\pi\sqrt{\frac{6D_\mu n}{K}}.$$

Remark. In a recent result of [35], Liu, Münch and Peyerimhoff proved a upper bound on the diameter under the weaker assumption $\mathrm{CD}(n, K)$ by using a different method.

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