BAKRY-ÉMERY CURVATURE FUNCTIONS OF GRAPHS

DAVID CUSHING, SHIPING LIU, AND NORBERT PEYERIMHOFF

Abstract. We study local properties of the Bakry-Émery curvature function $\mathcal{K}_{G,x} : (0, \infty] \to \mathbb{R}$ at a vertex x of a graph G systematically. Here $\mathcal{K}_{G,x}(\mathcal{N})$ is defined as the optimal curvature lower bound $\mathcal{K}$ in the Bakry-Émery curvature-dimension inequality $CD(\mathcal{K}, \mathcal{N})$ that x satisfies. We provide upper and lower bounds for the curvature functions, introduce fundamental concepts like curvature sharpness and S^1-out regularity, and relate the curvature functions of G with various spectral properties of (weighted) graphs constructed from local structures of G. We prove that the curvature functions of the Cartesian product of two graphs G_1, G_2 are equal to an abstract product of curvature functions of G_1, G_2. We explore the curvature functions of Cayley graphs and many particular (families of) examples. We present various conjectures and construct an infinite increasing family of 6-regular graphs which satisfy $CD(0, \infty)$ but are not Cayley graphs.

1. Introduction

In this section we introduce Bakry-Émery curvature and survey the main results of the paper.

A fundamental notion in the smooth setting of Riemannian manifolds is Ricci curvature. This notion has been generalized in various ways to the more general setting of metric spaces. In this article, we consider the discrete setting of graphs and study the optimal Ricci curvature lower bound $\mathcal{K}$ in Bakry-Émery's curvature-dimension inequality $CD(\mathcal{K}, \mathcal{N})$ at a vertex x of a graph G as a function of the variable $\mathcal{N} \in (0, \infty]$. Let us start to introduce this curvature notion which is based on the choice of a Laplace operator and which has been studied extensively in recent years (see, e.g., [35, 25, 20, 21, 10, 28, 18, 19]).

Let $G = (V, E)$ be a locally finite simple graph (that is, no loops and no multiple edges) with vertex set V and edge set E. For any $x, y \in V$, we write $x \sim y$ if $\{x, y\} \in E$. Let $d_x := \sum_{y: y \sim x} 1$ be the *degree of* x. We say a graph G is *d-regular* if $d_x = d$ for any $x \in V$. Let $\mathrm{dist} : V \times V \to \mathcal{N} \cup \{0\}$ denote the *combinatorial distance function*. For any function $f : V \to \mathbb{R}$ and any vertex $x \in V$, the *(non-normalized) Laplacian* Δ is defined via

$$\Delta f(x) := \sum_{y, y \sim x} (f(y) - f(x)). \tag{1.1}$$

The notion of a Laplacian can be generalised by intoducing a vertex measure and edge weights. In this article we will only consider curvature associated to the non-normalized Laplacian, except for the final Section 10, where we will briefly provide some additional information about this curvature notion for general Laplacians.

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Definition 1.1 (Γ and Γ_2 operators)**.** Let $G = (V, E)$ be a locally finite simple graph. For any two functions $f, g : V \to \mathbb{R}$, we define

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

We will write $\Gamma(f) := \Gamma(f,f)$ and $\Gamma_2(f,f) := \Gamma_2(f)$, for short.

Definition 1.2 (Bakry-Émery curvature)**.** Let $G = (V, E)$ be a locally finite simple graph. Let $\mathcal{K} \in \mathbb{R}$ and $\mathcal{N} \in (0, \infty]$. We say that a vertex $x \in V$ satisfies the *curvature-dimension inequality* $CD(\mathcal{K}, \mathcal{N})$, if for any $f : V \to \mathbb{R}$, we have

$$\Gamma_2(f)(x) \geq \frac{1}{\mathcal{N}}(\Delta f(x))^2 + \mathcal{K}\Gamma(f)(x). \tag{1.2}$$

We call $\mathcal{K}$ a lower Ricci curvature bound of x, and $\mathcal{N}$ a dimension parameter. The graph $G = (V, E)$ satisfies $CD(\mathcal{K}, \mathcal{N})$ (globally), if all its vertices satisfy $CD(\mathcal{K}, \mathcal{N})$. At a vertex $x \in V$, let $\mathcal{K}(G, x; \mathcal{N})$ be the largest $\mathcal{K}$ such that (1.2) holds for all functions f at x for a given $\mathcal{N}$. We call $\mathcal{K}_{G,x}(\mathcal{N}) := \mathcal{K}(G, x; \mathcal{N})$ the *Bakry-Émery curvature function* of x.

The reader can find various modifications of this curvature notion in, e.g., [5, 17, 30, 31, 26, 23]. It is natural to ask about the motivation for this curvature. The notion is rooted on *Bochner's formula*, a fundamental identity in Riemannian Geometry. The following remark explains this connection to the smooth setting in more detail.

Remark 1.3. Let $(M, \langle\cdot,\cdot\rangle)$ be a Riemannian manifold of dimension n with the Laplacian defined via $\Delta = \operatorname{div} \circ \operatorname{grad} \leq 0$.

Bochner's formula states for all smooth functions $f \in C^\infty(M)$ that

$$\frac{1}{2}\Delta|\operatorname{grad}\ f|^2(x) = |\operatorname{Hess}\ f|^2(x) + \langle \operatorname{grad}\ \Delta f(x), \operatorname{grad}\ f(x)\rangle + \operatorname{Ric}(\operatorname{grad}\ f(x)),$$

where Hess denotes the Hessian and Ric denotes the Ricci tensor. If $\operatorname{Ric}(v) \geq K_x|v|^2$ for all $v \in T_xM$ and, using the inequality $|\operatorname{Hess}\ f|^2(x) \geq \frac{1}{n}(\Delta f(x))^2$, we obtain

$$\frac{1}{2}\Delta|\operatorname{grad}\ f|^2(x) - \langle \operatorname{grad}\ \Delta f(x), \operatorname{grad}\ f(x)\rangle \geq \frac{1}{n}(\Delta f(x))^2 + K_x|\operatorname{grad}\ f(x)|^2.$$

The Γ and Γ_2 of Bakry-Émery [3] for two functions $f, g \in C^\infty(M)$ are defined as

$$\begin{aligned} 2\Gamma(f,g) &:= \Delta(fg) - f\Delta g - g\Delta f = \langle \operatorname{grad}\ f, \operatorname{grad}\ g\rangle, \\ 2\Gamma_2(f,g) &:= \Delta\Gamma(f,g) - \Gamma(f,\Delta g) - \Gamma(g,\Delta f). \end{aligned}$$

Noting that

$$\Gamma_2(f,f) = \frac{1}{2}\Delta|\operatorname{grad}\ f|^2 - \langle \operatorname{grad}\ \Delta f, \operatorname{grad}\ f\rangle$$

and by using Bochner's formula, we obtain the inequality

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

In conclusion, an n-dimensional Riemannian manifold $(M, \langle\cdot,\cdot\rangle)$ with Ricci curvature bounded below by K_x at $x \in M$ satisfies an inequality of the form given in (1.2). This suggests to use this inequality to define, indirectly, a Ricci curvature notion for a metric space via the help of the Laplacian.

Before we give a more detailed discussion of the results in this article, we like to first provide a rough overview with references to the sections:

- Section 2: Properties of Γ and Γ_2, by formulating curvature via semidefinite programming
- Section 4: General properties of curvature functions
- Sections 3 and 5: Upper and lower curvature bounds
- Section 6: Negative curvature at "bottlenecks"
- Section 7: Curvature of Cartesian products
- Section 8: Vertex curvature and spectral gaps in the 1-sphere.
- Section 9: Curvature of Cayley graphs and global $CD(0,\infty)$ conjectures
- Section 10: Curvature for graphs with general measures

1.1. **Properties of the Bakry-Émery curvature function.** In this article, we are particularly interested in the full Bakry-Émery curvature functions $\mathcal{K}_{G,x} : (0,\infty] \to \mathbb{R}$ at all vertices $x \in V$ which carry substantially more information than just the global $CD(\mathcal{K},\mathcal{N})$ condition. It follows directly from the definition that $\mathcal{K}_{G,x}$ is monotone non-decreasing. In fact, we study further properties of this curvature function in Section 4 and show that the function $\mathcal{K}_{G,x}$ is concave, continuous, and $\lim_{\mathcal{N}\to 0} K_{G,x}(\mathcal{N}) = -\infty$ (Proposition 4.1). Moreover, there exist constants $c_1(G,x), c_2(G,x)$, depending on the local structure at x, such that

$$c_1(G,x) - \frac{2d_x}{\mathcal{N}} \le \mathcal{K}_{G,x}(\mathcal{N}) \le c_2(G,x) - \frac{2d_x}{\mathcal{N}}. \tag{1.3}$$

The curvature function $\mathcal{K}_{G,x}$ is fully determined by the topology of the 2-ball $B_2(x) = \{y \in V : \mathrm{dist}(x,y) \le 2\}$ centered at $x \in V$ and Section 3 is concerned with the upper bound $c_2(G,x)$ in (1.3) in terms of this local structure. Introducing, for a vertex $y \in V$, the *out degree* (with respect to the center x)

$$d_y^{x,+} := |\{z : z \sim y, \mathrm{dist}(x,z) > \mathrm{dist}(x,y)\}|,$$

the *average out degree* $av_1^+(x)$ of the 1-sphere $S_1(x) := \{y \in V : \mathrm{dist}(x,y) = 1\}$ is defined by

$$av_1^+(x) = \frac{1}{d_x} \sum_{y \in S_1(x)} d_y^{x,+},$$

and the constant $c_2(G,)$ in (1.3) is given by (Theorem 3.1 and Definition 3.2)

$$c_2(G,x) = \mathcal{K}_\infty^0(x) := \frac{3 + d_x - av_1^+(x)}{2}. \tag{1.4}$$

Since, in many cases, the curvature function agrees with this upper bound, we introduce the following terminology:

Definition 1.4 (Curvature sharpness)**.** Let $G = (V,E)$ be a locally finite simple graph. Let $\mathcal{N} \in (0,\infty]$. We call a vertex $x \in V$ to be $\mathcal{N}$-*curvature sharp* if $\mathcal{K}_{G,x}(\mathcal{N})$ agrees with the upper bound given in (1.3) and (1.4), that is

$$\mathcal{K}_{G,x}(\mathcal{N}) = \mathcal{K}_\infty^0(x) - \frac{2d_x}{\mathcal{N}}.$$

We call the graph G to be $\mathcal{N}$-curvature sharp, if every vertex $x \in V$ is $\mathcal{N}$-curvature sharp.

We will show that if x is $\mathcal{N}$-curvature sharp, then it is also $\mathcal{N}'$-curvature for all smaller values $\mathcal{N}'$ (Proposition 4.6). Moreover, monotonicity and concavity of $\mathcal{K}_{G,x}$ imply that if $\mathcal{K}_{G,x}(\mathcal{N}_1) = \mathcal{K}_{G,x}(\mathcal{N}_2)$ for $\mathcal{N}_1 < \mathcal{N}_2$, then $\mathcal{K}_{G,x}(\mathcal{N})$ is constant for all values $\mathcal{N} \ge \mathcal{N}_1$ (Proposition 4.5).

A natural question is what local information can be extracted from the curvature function $\mathcal{K}_{G,x}$. We show that the degree d_x can be read off via (Corollary 4.4)

$$d_x = -\frac{1}{2} \lim_{\mathcal{N}\to 0} \mathcal{N}\mathcal{K}_{G,x}(\mathcal{N}),$$

and the average out-degree $av_1^+(x)$ can be read off via (Corollary 5.6)

$$av_1^+ = 3 + d_x - 2 \lim_{\mathcal{N}\to 0} \left(\mathcal{K}_{G,x}(\mathcal{N}) + \frac{2d_x}{\mathcal{N}} \right).$$

Proposition 4.1 also provides the lower curvature bound $c_1(G,x) = \mathcal{K}_{G,x}(\infty)$ in (1.3). Section 5 provides another lower curvature bound in terms of the upper bound (1.4) and a correction term given by the (non-positive) smallest eigenvalue of a specific matrix $\widehat{\mathcal{P}}_{\mathcal{N}}$ (Theorem 5.5).

1.2. **Curvature of S_1-out regular vertices.** Now we introduce a certain homogeneity property within the 2-ball of a vertex, called S_1*-out regularity.* It turns out that this notion is closely linked to the curvature sharpness introduced above.

Definition 1.5 (S_1-out regularity)**.** We say a locally finite simple graph G is S_1*-out regular* at x, if all vertices in $S_1(x)$ have the same out degree.

We have the following surprising characterization: A graph G is S_1-out regular at a vertex x if and only if there exists $\mathcal{N} \in (0,\infty]$ such that x is $\mathcal{N}$-curvature sharp (Corollary 5.10). That is, the curvature function $\mathcal{K}_{G,x}$ assumes the upper bound $\mathcal{K}^0_\infty(x) - 2d_x/\mathcal{N}$ for some $\mathcal{N} \in (0,\infty]$ if and only if the local structure around x is homogeneous in the sense of S_1-out regularity. Moreover, when G is S_1-out regular at x, there exists a threshold $\mathcal{N}_0(x)$ such that x is $\mathcal{N}$-curvature sharp for any $\mathcal{N} \in (0, \mathcal{N}_0(x)]$, and $\mathcal{K}_{G,x}(\mathcal{N}) \equiv \mathcal{K}_{G,x}(\mathcal{N}_0(x))$ for any $\mathcal{N} \in [\mathcal{N}_0(x), \infty]$ (Theorem 5.7).

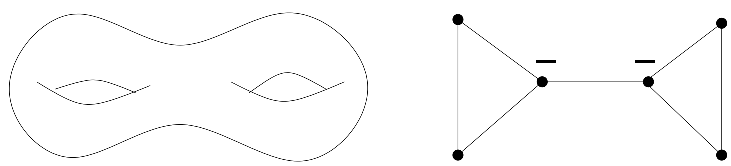

FIGURE 1. Negative curvature at a "bottleneck"

1.3. **Curvature and local connectedness.** A well know phenomenon in the setting of Riemannian surfaces is that "bottlenecks" generate regions of negative curvature. A similar phenomenon occurs in the graph setting (the two vertices at the bottleneck in Figure 1 have strictly negative curvature functions). More generally, the curvature $\mathcal{K}_{G,x}(\infty)$ is – with very few exceptions – always negative, if the *punctured* 2*-ball* $\mathring{B}_2(x) = B_2(x) - \{x\}$ has more than one connected component (Theorem 6.4). Here $\mathring{B}_2(x)$ denotes the subgraph containing all spherical edges of $S_1(x)$ and all radial edges between $S_1(x)$ and the 2-sphere $S_2(x)$ (but not the radial edges of $S_2(x)$, since they have no influence on the curvature function at x). Further relations between the curvature and the local structure of $\mathring{B}_2(x)$ will be presented in Section 6. In the specific case of an S_1-out regular vertex $x \in V$ with $\mathring{B}_2(x)$ having more than one connected component, we derive in Section 8 the explicit expression $\mathcal{K}_{G,x}(\infty) = (3 - d_x - av_1^+)/2$, which is negative as soon as $d_x + av_1^+ > 3$ (Corollary 8.4). This follows from a precise formula for the curvature function $\mathcal{K}_{G,x}$ in terms of the spectral gap of a weighted graph $S_1''(x)$ of size d_x constructed from $\mathring{B}_2(x)$ (Theorem 8.1) in the specific case of an S_1-regular vertex x.

1.4. **Curvature of Cartesian products.** In Section 7, we discuss curvature functions of Cartesian products. Let $G_i = (V_i, E_i)$ be two locally finite simple graphs and let $x \in V_1, y \in V_2$. Then the curvature function $\mathcal{K}_{G_1 \times G_2,(x,y)}$, $(x, y) \in V_1 \times V_2$ is gvien by

$$\mathcal{K}_{G_1 \times G_2,(x,y)}(\mathcal{N}) = \mathcal{K}_{G_1,x}(\mathcal{N}_1) = \mathcal{K}_{G_2,y}(\mathcal{N}_2),$$

where $\mathcal{N}_1, \mathcal{N}_2 > 0$ are chosen such that $\mathcal{N} = \mathcal{N}_1 + \mathcal{N}_2$ and $\mathcal{K}_{G_1,x}(\mathcal{N}_1) = \mathcal{K}_{G_2,y}(\mathcal{N}_2)$. We say that $\mathcal{K}_{G_1 \times G_2,(x,y)}$ is the $*$-product of $\mathcal{K}_{G_1,x}$ and $\mathcal{K}_{G_2,y}$. This $*$-product (Definition 7.1) of the curvature functions is a well-defined abstract product and interesting in its own right. In Figure 2, we illustrate the curvature functions of the complete graphs K_2 and K_3 and their Cartesian product $K_2 \times K_3$. Observe that $\mathcal{K}_{K_2}(4) = \mathcal{K}_{K_3}(4) = 3/2$. As illustrated in Figure 3, this tells us that $\mathcal{K}_{K_2 \times K_3}(8) = 3/2$.

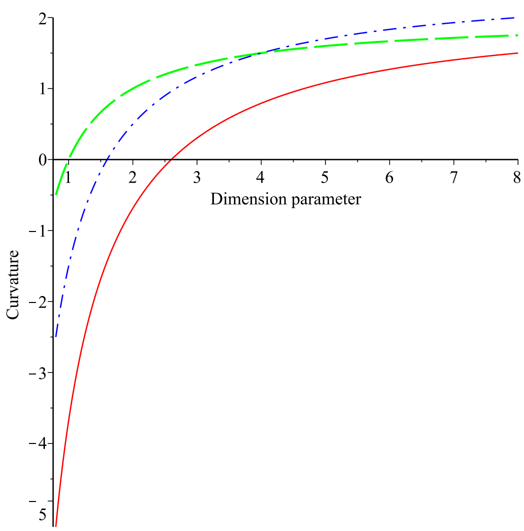

FIGURE 2. Curvature functions of $\mathcal{K}_{K_2}(\mathcal{N})$ (dashed), $\mathcal{K}_{K_3}(\mathcal{N})$ (dashdotted), and $\mathcal{K}_{K_2 \times K_3}(\mathcal{N})$ (solid) when $\mathcal{N} \in [0.8, 8]$.

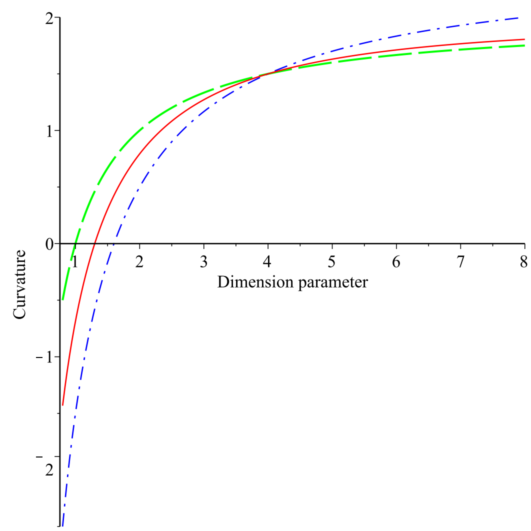

FIGURE 3. Curvature functions of $\mathcal{K}_{K_2}(\mathcal{N})$ (dashed), $\mathcal{K}_{K_3}(\mathcal{N})$ (dashdotted), and $\mathcal{K}_{K_2 \times K_3}(2\mathcal{N})$ (solid) when $\mathcal{N} \in [0.8, 8]$.

1.5. **Curvature of specific graph families.** We calculate curvature functions of many particular graph families, e.g.,

- paths and cycles, star graphs and regular trees, complete graphs, complete bipartite graphs, and crown graphs in Section 5.3,
- hypercubes and line graphs of bipartite graphs in Section 7.3,
- and Johnson graphs in Example 8.7.

In Section 9, we study curvature functions of *Cayley graphs*. It is well know that all abelian Cayley graphs satisfy the $CD(0, \infty)$ condition. In Theorem 9.6, we give a direct relation between the curvature function of the Cayley graph of a Coxeter group with standard generators (which can be huge; for example, the Cayley graph of E_8 is of size $192 \cdot 10!$) and the maximal eigenvalue of the Laplacian of the corresponding Coxeter diagram (which is usually very small in comparison; in the example E_8 of size 8).

It is not known and a very interesting question whether there exist infinite expander families in the class $CD(0,\infty)$ or not (Conjecture 9.11). Such an expander family cannot consist of *abelian* Cayley graphs. In Example 9.12 we construct an infinite family of increasing 6-regular non-Cayley graphs satisfying $CD(0,\infty)$, but it is easy to see that this class is not a family of expanders.

1.6. **Return to Riemannian manifolds.** Readers not interesting in the Riemannian manifold case can safely skip this subsection, which draws a comparison between curvature functions of graphs with that of weighted Riemannian manifolds.

A *weighted Riemannian manifold* is a triple $(M^n, g, e^{-f}d\mathrm{vol}_g)$, where (M^n, g) is an n-dimensional complete Riemannian manifold, $d\mathrm{vol}_g$ is the Riemannian volume element, and f is a smooth real valued function on M^n. The $\mathcal{N}$-dimensional weighted Ricci tensor of $(M^n, g, e^{-f}d\mathrm{vol}_g)$ is

$$\mathrm{Ric}_f(\mathcal{N}) := \mathrm{Ric} + \mathrm{Hess}f - \frac{df \otimes df}{\mathcal{N} - n}, \tag{1.5}$$

where Ric is the Ricci curvature tensor of (M^n, g), Hess$f$ is the Hessian of f ([3, 34]). Using the f-Laplacian $\Delta_f = \Delta_g - \nabla f \cdot \nabla$, where Δ_g is the Laplace-Beltrami operator on (M^n, g), one can define the Bakry-Émery curvature-dimension inequality $CD(\mathcal{K},\mathcal{N})$ as in Definitions 1.1 and 1.2. Then $CD(\mathcal{K},\mathcal{N}), \mathcal{N} \in (n,\infty]$ holds if and only if $\mathrm{Ric}_f(\mathcal{N}) \geq \mathcal{K}$ (see, e.g., [2, Section 3]). Recall n in (1.5) is the dimension of the underlying Riemannian manifold. When f is not constant, the lower bound of $\mathrm{Ric}_f(\mathcal{N})$ tends to $-\infty$ as $\mathcal{N}$ tends to n. So, in comparison, a graph can be considered as 0-dimensional. This is natural in the sense that we are using a difference operator to define the curvature functions of a graph.

Recently, the conditions $\mathrm{Ric}_f(\mathcal{N}) \geq \mathcal{K}$ on $(M^n, g, e^{-f}d\mathrm{vol}_g)$, where $\mathcal{N} < n$, have also been studied in [22, 32]. In particular, for $\mathcal{N} \in (-\infty, n)$, $CD(\mathcal{K},\mathcal{N})$ holds if and only if $\mathrm{Ric}_f(\mathcal{N}) \geq \mathcal{K}$ ([22, Remark 2.4], [32, Theorem 4.10]). In principle, the curvature functions of a graph studied in this article can also be defined on $(-\infty, 0) \cup (0,\infty]$. However, we will restrict ourselves to curvature functions on the interval $(0,\infty]$.

2. Bakry-Émery curvature and local Γ and Γ_2 matrices

In this section, we view curvature as solution of a *semidefinite programming problem* and derive upper curvature bounds via higher multiplicities of the zero eigenvalue of certain matrices. We also derive some properties of vertices satisfying the $CD(0,\mathcal{N})$ condition.

2.1. **Fundamental notions.** Henceforth, we use the standard notation $[k] := \{1, 2, \dots, k\}$. Given a vertex $x \in V$, the curvature function $\mathcal{K}_{G,x}$ only depends on the local structure of the graph around x. We now prepare the notations describing this local structure. We denote by dist the discrete graph distance. For any $r \in \mathbb{N}$, the r-ball centered at x is defined as

$$B_r(x) := \{y \in V : \mathrm{dist}(x, y) \leq r\},$$

and the r-sphere centered at x is

$$S_r(x) := \{y \in V : \mathrm{dist}(x, y) = r\}.$$

Then we have the following decomposition of the 2-ball $B_2(x)$:

$$B_2(x) = \{x\} \sqcup S_1(x) \sqcup S_2(x).$$

We call an edge $\{y,z\}\in E$ a *spherical edge* (w.r.t. x) if $\mathrm{dist}(x,y)=\mathrm{dist}(x,z)$, and a *radial edge* if otherwise. For a vertex $y\in V$, we define

$$\begin{aligned} d_y^{x,+} &:= |\{z : z\sim y, \mathrm{dist}(x,z)>\mathrm{dist}(x,y)\}|,\\ d_y^{x,0} &:= |\{z : z\sim y, \mathrm{dist}(x,z)=\mathrm{dist}(x,y)\}|,\\ d_y^{x,-} &:= |\{z : z\sim y, \mathrm{dist}(x,z)<\mathrm{dist}(x,y)\}|. \end{aligned}$$

In the above, the notation $|\cdot|$ stands for the cardinality of the set. We call $d_y^{x,+}$, $d_y^{x,0}$, and $d_y^{x,-}$ the *out degree*, *spherical degree*, and *in degree* of y w.r.t. x. We sometimes write d_y^+, d_y^0, d_y^- for short when the reference vertex x is clear from the context.

By abuse of notion, we use $S_1(x)$ in this article also for the induced subgraph of the vertices in $S_1(x)$ in a graph G; we use $B_2(x)$ also for the subgraph of G with vertex set $B_2(x)$ and edge set given by the radial edges connecting $\{x\}$ and $S_1(x)$, the radial edges between $S_1(x)$ and $S_2(x)$, and the spherical edges in $S_1(x)$. Note that this graph is not the induced subgraph of $B_2(x)$ in G (since the spherical edges in $S_2(x)$ are not included), but this local information is all that is needed for the calculation of the Bakry-Émery curvature function $\mathcal{K}_{G,x}$. We denote by $\mathring{B}_2(x)$ the subgraph of $B_2(x)$ obtained by deleting $\{x\}$ and all radial edges connecting $\{x\}$ and $S_1(x)$.

Since at a vertex x, both $\Gamma(f,g)(x)$ and $\Gamma_2(f,g)(x)$ are quadratic forms, we can talk about their local matrices. The curvature-dimension inequalities can be reformulated as linear matrix inequalities. Recall the following proposition (see [26, Proposition 3.10]).

Proposition 2.1 ([26])**.** *Let $G=(V,E)$ be a locally finite simple graph and let $x\in V$. The Bakry-Émery curvature function $\mathcal{K}_{G,x}(\mathcal{N})$ valued at $\mathcal{N}\in(0,\infty]$ is the solution of the following semidefinite programming,*

$$\begin{aligned} &\textit{maximize } K\\ &\textit{subject to } \Gamma_2(x)-\frac{1}{\mathcal{N}}\Delta(x)^\top\Delta(x)\geq K\Gamma(x), \end{aligned}$$

In the above, the local matrices $\Gamma_2(x)$, $\Delta(x)$, and $\Gamma(x)$ are matrices of sizes $|V|$ by $|V|$, 1 by $|V|$, and $|V|$ by $|V|$, respectively. But their non-trivial blocks are of relatively small sizes. For example, the non-trivial block of $\Delta(x)$ is the one corresponding to vertices $B_1(x)$ given by

$$\Delta(x)=\begin{pmatrix}-d_x & 1 & \cdots & 1\end{pmatrix}, \tag{2.1}$$

It is of size 1 by $|B_1(x)|=d_x+1$. The non-trivial blocks of $\Gamma(x)$ and $\Gamma_2(x)$ are of sizes $|B_2(x)|$ by $|B_2(x)|$ and $|B_1(x)|$ by $|B_1(x)|$, respectively. In the remaining part of this paper, we will reserve the notations $\Gamma_2(x)$, $\Delta(x)$, and $\Gamma(x)$ for their non-trivial block. Whenever we write linear combinations of them, we pad matrices of smaller sizes with 0 entries.

We will discuss the local matrices $\Gamma(x)$ and $\Gamma_2(x)$ in more details in the following subsections.

2.2. **Local Γ matrix and its basic properties.** We check by definition that $\Gamma(x)$ is a $|B_1(x)|$ by $|B_1(x)|$ matrix corresponding to vertices in $B_1(x)$ given by

$$2\Gamma(x)=\begin{pmatrix} d_x & -1 & \cdots & -1\\ -1 & 1 & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ -1 & 0 & \cdots & 1 \end{pmatrix}. \tag{2.2}$$

The following property is a direct observation. Let us denote by $\mathbf{1}_{d_x+1} := (1, 1, \ldots, 1)^\top$ and by $\mathbf{1}_{d_x+1}^\perp$ the orthogonal complement of the subspace spanned by $\mathbf{1}_{d_x+1}$ in $\mathbb{R}^{d_x+1}$. For convenience, we will often drop the subindex when no confusion is possible.

Proposition 2.2. *Let $v \in \mathbb{R}^{d_x+1}$. Then $\Gamma(x)v = 0$ if and only if $v = a\mathbf{1}$ for some constant $a \in \mathbb{R}$. Moreover, the smallest eigenvalue $\lambda_{\min}(2\Gamma(x)|_{\mathbf{1}^\perp})$ of $2\Gamma(x)$ restricted to the subspace $\mathbf{1}^\perp$ satisfies*

$$\lambda_{\min}(2\Gamma(x)|_{\mathbf{1}^\perp}) \geq 1. \tag{2.3}$$

The equality holds in (2.3) when $d_x > 1$.

Proof. By (2.2), $2\Gamma(x)$ is diagonal dominant and $2\Gamma(x)\mathbf{1} = 0$.

For any $v := (v_0, v_1, \ldots, v_{d_x})^\top \in \mathbf{1}^\perp$, we have $v_0 = -\sum_{i=1}^{d_x} v_i$, and therefore,

$$v^\top(2\Gamma(x))v = (d_x+1)v_0^2 + \sum_{i=0}^{d_x} v_i^2 \geq |v|^2, \tag{2.4}$$

where $|v|$ is the norm of v. This shows $\lambda_{\min}(2\Gamma(x)|_{\mathbf{1}^\perp}) \geq 1$.

When $d_x > 1$, there exists $v := (v_0, v_1, \ldots, v_{d_x})^\top \in \mathbf{1}^\perp$ with $v_0 = 0$. We can check

$$2\Gamma(x)v = v.$$

Hence in this case $\lambda_{\min}(2\Gamma(x)|_{\mathbf{1}^\perp}) = 1$. □

2.3. **Local Γ_2 matrix and its basic properties.** The matrix $\Gamma_2(x)$ is of size $|B_2(x)| \times |B_2(x)|$ with the following structure ([26, Proposition 3.12])

$$4\Gamma_2(x) = \begin{pmatrix} (4\Gamma_2(x))_{x,x} & (4\Gamma_2(x))_{x,S_1(x)} & (4\Gamma_2(x))_{x,S_2(x)} \\ (4\Gamma_2(x))_{S_1(x),x} & (4\Gamma_2(x))_{S_1(x),S_1(x)} & (4\Gamma_2(x))_{S_1(x),S_2(x)} \\ (4\Gamma_2(x))_{S_2(x),x} & (4\Gamma_2(x))_{S_2(x),S_1(x)} & (4\Gamma_2(x))_{S_2(x),S_2(x)} \end{pmatrix}. \tag{2.5}$$

The sub-indices indicate the vertices that each submatrix is corresponding to. We will omit the dependence on x in the above expressions for simplicity. When we exchange the order of the sub-indices, we mean the transpose of the original submatrix. For example, we have $(4\Gamma_2)_{S_1,x} := ((4\Gamma_2)_{x,S_1})^\top$.

Denote the vertices in $S_1(x)$ by $\{y_1, \ldots, y_{d_x}\}$. Then we have

$$(4\Gamma_2)_{x,x} = 3d_x + d_x^2, \quad (4\Gamma_2)_{x,S_1} = \begin{pmatrix} -3 - d_x - d_{y_1}^+ & \cdots & -3 - d_x - d_{y_{d_x}}^+ \end{pmatrix}, \tag{2.6}$$

and

$$\begin{aligned} &(4\Gamma_2)_{S_1,S_1} \\ &= \begin{pmatrix} 5 - d_x + 3d_{y_1}^+ + 4d_{y_1}^0 & 2 - 4w_{y_1y_2} & \cdots & 2 - 4w_{y_1y_{d_x}} \\ 2 - 4w_{y_1y_2} & 5 - d_x + 3d_{y_2}^+ + 4d_{y_2}^0 & \cdots & 2 - 4w_{y_2y_{d_x}} \\ \vdots & \vdots & \ddots & \vdots \\ 2 - 4w_{y_1y_{d_x}} & 2 - 4w_{y_2y_{d_x}} & \cdots & 5 - d_x + 3d_{y_{d_x}}^+ + 4d_{y_{d_x}}^0 \end{pmatrix}, \end{aligned} \tag{2.7}$$

where we use the notation that for any two vertices $x, y \in V$,

$$w_{xy} = \begin{cases} 1, & \text{if } x \sim y \\ 0, & \text{otherwise.} \end{cases} \tag{2.8}$$

Denote the vertices in $S_2(x)$ by $\{z_1, \ldots, z_{|S_2(x)|}\}$. Then we have

$$(4\Gamma_2)_{x,S_2} = \begin{pmatrix} d_{z_1}^- & d_{z_2}^- & \cdots & d_{z_{|S_2(x)|}}^- \end{pmatrix}, \tag{2.9}$$

$$(4\Gamma_2)_{S_1,S_2} = \begin{pmatrix} -2w_{y_1z_1} & -2w_{y_1z_2} & \cdots & -2w_{y_1z_{|S_2(x)|}} \\ \vdots & \vdots & \ddots & \vdots \\ -2w_{y_{d_x}z_1} & -2w_{y_{d_x}z_2} & \cdots & -2w_{y_{d_x}z_{|S_2(x)|}} \end{pmatrix}. \tag{2.10}$$

and

$$(4\Gamma_2)_{S_2,S_2} = \begin{pmatrix} d^-_{z_1} & 0 & \cdots & 0 \\ 0 & d^-_{z_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d^-_{z_{|S_2(x)|}} \end{pmatrix}. \tag{2.11}$$

Note that each diagonal entry of $(4\Gamma_2)_{S_2,S_2}$ is positive.

Let $A(G)$ be the adjacency matrix of the graph G. Then we see

$$(4\Gamma_2)_{S_1,S_2} = -2 \cdot A(G)_{S_1,S_2}.$$

In fact, we can decompose the matrix $4\Gamma_2$ as follows:

$$4\Gamma_2 = \left(\begin{array}{c|c|c} 0 & 0 & 0 \\ \hline 0 & -4\,\Delta|_{S_1(x)} & 0 \\ \hline 0 & 0 & 0 \end{array}\right) + \left(\begin{array}{c|cc} 0 & 0 & 0 \\ \hline 0 & & \\ 0 & \multicolumn{2}{c}{-2\,\Delta|_{\mathring{B}_2(x)}} \end{array}\right)$$

$$+ \left(\begin{array}{c|ccc|ccc} 3d_x + d_x^2 & -3 - d_x - d^+_{y_1} & \cdots & -3 - d_x - d^+_{y_{d_x}} & d^-_{z_1} & \cdots & d^-_{z_{|S_2|}} \\ \hline -3 - d_x - d^+_{y_1} & 5 - d_x + d^+_{y_1} & \cdots & 2 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ -3 - d_x - d^+_{y_{d_x}} & 2 & \cdots & 5 - d_x + d^+_{y_{d_x}} & 0 & \cdots & 0 \\ \hline d^-_{z_1} & 0 & \cdots & 0 & -d^-_{z_1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ d^-_{z_{|S_2|}} & 0 & \cdots & 0 & 0 & \cdots & -d^-_{z_{|S_2|}} \end{array}\right).$$

In the above, $\Delta|_{S_1(x)}$ and $\Delta|_{\mathring{B}_2(x)}$ are the non-normalized Laplacian of the subgraphs $S_1(x)$ and $\mathring{B}_2(x)$, respectively.

The following proposition can be checked directly.

Proposition 2.3. *For the constant vector* $\mathbf{1} \in \mathbb{R}^{|B_2(x)|}$*, we have* $\Gamma_2(x)\mathbf{1} = 0$.

2.4. **Multiplicity of zero eigenvalue of $\Gamma_2(x)$ and curvature.** By Proposition 2.3, the multiplicity of zero eigenvalue of matrix $\Gamma_2(x)$ is at least one. In this subsection, we discuss an interesting relation between this multiplicity and the curvature at x.

Theorem 2.4. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$ be a vertex. If the multiplicity of the zero eigenvalue of $\Gamma_2(x)$ is at least 2, then we have $\mathcal{K}_{G,x}(\infty) \leq 0$.*

Let us first show the following lemma.

Lemma 2.5. *Let* $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ *with* $v_1 \in \mathbb{R}^{|B_1(x)|}$ *and* $v_2 \in \mathbb{R}^{|S_2(x)|}$ *be a non-constant vector such that* $\Gamma_2(x)v = 0$*. Then we have* $\Gamma(x)v_1 \neq 0$.

Proof. We prove the lemma by contradiction. Assume that $\Gamma(x)v_1 = 0$. By Proposition 2.2, we have

$$v_1 = a\mathbf{1}_{|B_1(x)|}, \quad \text{for some} \quad a \in \mathbb{R}. \tag{2.12}$$

Let us denote

$$w := a\mathbf{1}_{|S_2(x)|} - v_2 = \begin{pmatrix} 0 \\ a\mathbf{1}_{|B_1(x)|} - v_2 \end{pmatrix}.$$

Then by Proposition 2.3, we have $\Gamma_2(x)w = 0$.

Since the submatrix $(\Gamma_2)_{S_2,S_2}$ is invertible (recall (2.11)), we conclude that

$$v_2 = a\mathbf{1}_{|B_1(x)|}. \tag{2.13}$$

(2.12) and (2.13) imply that v_2 is a constant vector, which is a contradiction. □

Proof of Theorem 2.4. We argue by contradiction. Suppose that $K := \mathcal{K}_{G,x}(\infty) > 0$. Then we have

$$\Gamma_2(x) - K\Gamma(x) \geq 0. \tag{2.14}$$

By assumption, there exists a non-constant vector $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ such that

$$v^T\Gamma_2(x)v = 0. \tag{2.15}$$

Applying Lemma 2.5, we obtain from (2.14)

$$v^T\Gamma_2(x)v \geq Kv_1^T\Gamma(x)v_1 > 0, \tag{2.16}$$

which is a contradiction to (2.15). □

For any $\mathcal{N} \in (0,\infty]$ and $K \in \mathbb{R}$, we denote

$$M_{K,\mathcal{N}}(x) := \Gamma_2(x) - \frac{1}{\mathcal{N}}\Delta(x)^\top\Delta(x) - K\Gamma(x), \tag{2.17}$$

Observe that $M_{K,\mathcal{N}}(x)\mathbf{1} = 0$, and its (S_2, S_2)-block, which equals $(\Gamma_2)_{S_2,S_2}$, is invertible. Therefore, from the above proofs, it is not hard to see analogous result of Theorem 2.4 also holds for $M_{K,\mathcal{N}}$.

Theorem 2.6. *Let $G = (V,E)$ be a locally finite simple graph and $x \in V$ be a vertex. Let $\mathcal{N} \in (0,\infty]$ and $K \in \mathbb{R}$. If the multiplicity of the zero eigenvalue of the matrix $M_{K,\mathcal{N}}$ is at least 2, then we have $\mathcal{K}_{G,x}(\mathcal{N}) \leq K$.*

The following result is an immediate consequence of Theorem 2.6.

Corollary 2.7. *Let $G = (V,E)$ be a locally finite simple graph and $x \in V$ be a vertex. Let $\mathcal{N} \in (0,\infty]$ and $K \in \mathbb{R}$. Then the following are equivalent:*

(i) *$\mathcal{K}_{G,x}(\mathcal{N}) = K$;*

(ii) *The matrix $M_{K,\mathcal{N}}(x) \geq 0$ and the multiplicity of its zero eigenvalue is at least 2.*

Proof. (ii) ⇒ (i): Since $M_{K,\mathcal{N}}(x) \geq 0$, we have $\mathcal{K}_{G,x}(\mathcal{N}) \geq K$. By Theorem 2.6, (ii) implies $\mathcal{K}_{\mathcal{N}}(G,x) \leq K$. Therefore, we obtain $\mathcal{K}_{\mathcal{N}}(G,x) = K$.

(i) ⇒ (ii): (i) implies $M_{K,\mathcal{N}} \geq 0$ immediately. Assume that the zero eigenvalue of $M_{K,\mathcal{N}}(x)$ has multiplicity 1. Then the smallest eigenvalue $\lambda_{\min}(M_{K,\mathcal{N}}(x)|_{\mathbf{1}^\perp})$ of $M_{K,\mathcal{N}}$ restricted to the space $\mathbf{1}^\perp$ is positive. Let $\lambda_{\max}(\Gamma(x))$ be the maximal eigenvalue of $\Gamma(x)$. We observe that

$$M_{K,\mathcal{N}}(x) - \epsilon\Gamma(x) \geq 0, \text{ for any } 0 < \epsilon < \frac{\lambda_{\max}(\Gamma(x))}{\lambda_{\min}(M_{K,\mathcal{N}}(x)|_{\mathbf{1}^\perp})}, \tag{2.18}$$

which is a contradiction to (i). □

2.5. **Vertices satisfying $CD(0,\mathcal{N})$.** In this subsection, we discuss immediate properties of a vertex x satisfying $CD(0,\mathcal{N})$, by considering two particular principal minors of the matrix $M_{0,\mathcal{N}}(x)$: the determinants of (x,x)- and $(B_1(x),B_1(x))$- blocks.

Proposition 2.8. *Let $G=(V,E)$ be a locally finite simple graph and $x\in V$. If x satisfies $CD(0,\mathcal{N})$, then we have*

$$\frac{4d_x}{d_x+3}\leq\mathcal{N}. \tag{2.19}$$

Proof. By Corollary 2.7, we have $4M_{0,\mathcal{N}}(x)\geq 0$. From Sylvester's criterion we have

$$(4M_{0,\mathcal{N}}(x))_{x,x}=3d_x+d_x^2-\frac{4d_x^2}{\mathcal{N}}\geq 0.$$

Rearranging we thus obtain (2.19). □

Proposition 2.8 has interesting consequences.

Corollary 2.9. *Let $G=(V,E)$ be a locally finite simple graph and let $x\in V$. Then $\mathcal{K}_{G,x}(\mathcal{N})<0$ when $\mathcal{N}<1$.*

Proof. Let $\mathcal{N}<1$. Assume that $\mathcal{K}_{G,x}(\mathcal{N})\geq 0$. Then by Proposition 2.8, we have $4d_x<3d_x+1$. Hence $d_x<1$, which is impossible. □

Remark 2.10. Corollary 2.9 can also be shown by Lichnerowicz type estimate, see [26, Corollary 6.2].

Corollary 2.11. *Let $G=(V,E)$ be a locally finite simple graph satisfying $CD(0,\mathcal{N})$. Let $d_{\max}$ denote the maximum degree taken over all vertices. Then*

- *If $\mathcal{N}\in(0,4)$ then $d_{\max}\leq\frac{3\mathcal{N}}{4-\mathcal{N}}$.*
- *If $\mathcal{N}=4$ then $d_{\max}$ may be arbitrarily large.*

Proof. The case $\mathcal{N}\in(0,4)$ is obtained directly from Proposition 2.8. For $\mathcal{N}=4$, consider the complete graphs K_n on n vertices which satisfy $CD(0,4)$ (see, e.g., [20, Proposition 3] or Example 5.17). □

Proposition 2.12. *Let $G=(V,E)$ be a locally finite simple graph. For a vertex $x\in V$, let us denote*

$$c_1(x):=\det\left(\Gamma_2(x)_{B_1,B_1}\right)\ \text{and}\ c_2(x)=\Delta(x)\mathrm{adj}\left(\Gamma_2(x)_{B_1,B_1}\right)\Delta(x)^\top,$$

where $\mathrm{adj}(\cdot)$ stands for the adjugate matrix. If x satisfies $CD(0,\mathcal{N})$, then we have

$$c_1(x)\geq\frac{c_2(x)}{\mathcal{N}}.$$

Proof. By assumption, we have $M_{0,\mathcal{N}}(x)\geq 0$. From Sylvester's criterion we have

$$\det\left(\Gamma_2(x)_{B_1,B_1}-\frac{1}{\mathcal{N}}\Delta(x)^\top\Delta(x)\right)\geq 0.$$

Applying the Matrix Determinant Lemma, we obtain

$$\det\left(\Gamma_2(x)_{B_1,B_1}\right)-\frac{1}{\mathcal{N}}\Delta(x)\mathrm{adj}\left(\Gamma_2(x)_{B_1,B_1}\right)\Delta(x)^\top\geq 0.$$

This completes the proof. □

Example 2.13 ($K_{2,6}$)**.** Consider the complete bipartite graph $K_{2,6}$. Let x be a vertex with degree 2. Then we can check

$$\Gamma_2(x)_{B_1,B_1} = \frac{1}{2}\begin{pmatrix} 5 & -5 & -5 \\ -5 & 9 & 1 \\ -5 & 1 & 9 \end{pmatrix}, \text{ and } \Delta(x) = \begin{pmatrix} -2 & 1 & 1 \end{pmatrix}.$$

Hence, we have $c_1(x) = 0$ and $c_2(x) = 20$. By Proposition 2.12, we know, for any finite $\mathcal{N} > 0$, that x does not satisfy $CD(0, \mathcal{N})$. However, we will show that the graph $K_{2,6}$ satisfies $CD(0, \infty)$.

In Section 3, we will derive interesting upper curvature bound by considering the $(\{x\} \sqcup S_2(x), \{x\} \sqcup S_2(x))$-minor of $M_{K,\mathcal{N}}(x)$.

3. An upper curvature bound

In this section, we derive an upper bound on Bakry-Émery curvature function $\mathcal{K}_{G,x}$ in terms of the local topological structure around x (Theorem 3.1). Let us denote the average degree and average out-degree of $S_1(x)$ by

$$av_1(x) := \frac{1}{d_x} \sum_{y \in S_1(x)} d_y, \quad \text{and} \quad av_1^+(x) := \frac{1}{d_x} \sum_{y \in S_1(x)} d_y^+ \tag{3.1}$$

We write $d_y^0 = \#_\Delta(x, y)$ alternatively to emphasis its geometric meaning: It is the number of triangles (3-cycles) including the edge $\{x, y\}$. We have

$$\sum_{y \in S_1(x)} d_y^0 = \sum_{y \in S_1(x)} \#_\Delta(x, y) =: 2\#_\Delta(x), \tag{3.2}$$

where $\#_\Delta(x)$ is the number of triangles including the vertex x.

Theorem 3.1. *Let $G = (V, E)$ be a locally finite simple graph and let $x \in V$. For $\mathcal{N} \in (0, \infty]$, we have*

$$K_{G,x}(\mathcal{N}) \leq 2 + \frac{d_x - av_1(x)}{2} + \frac{\#_\Delta(x)}{d_x} - \frac{2d_x}{\mathcal{N}}. \tag{3.3}$$

Proof. Let $\mathcal{K} := \mathcal{K}_{G,x}(\mathcal{N})$. Then the matrix

$$4M_{\mathcal{K},\mathcal{N}}(x) = 4\left(\Gamma_2(x) - \frac{1}{\mathcal{N}}\Delta(x)^\top \Delta(x) - \mathcal{K}\Gamma(x)\right) \geq 0.$$

Let M_0 be the submatrix corresponding to the vertices $\{x\} \sqcup S_2(x) = \{x, z_1, \ldots, z_{|S_2(x)|}\}$. The matrix M_0 has the form

$$M_0 = \begin{pmatrix} d_x^2 + 3d_x - 2\mathcal{K}d_x - \frac{4d_x^2}{\mathcal{N}} & d_{z_1}^- & d_{z_2}^- & \cdots & d_{z_{|S_2(x)|}}^- \\ d_{z_1}^- & d_{z_1}^- & 0 & \cdots & 0 \\ d_{z_2}^- & 0 & d_{z_2}^- & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ d_{z_{|S_2(x)|}}^- & 0 & 0 & \cdots & d_{z_{|S_2(x)|}}^- \end{pmatrix}. \tag{3.4}$$

We have, by Sylvester's criterion, $det(M_0) \geq 0$. Thus

$$d_x^2 + 3d_x - 2\mathcal{K}d_x - \frac{4d_x^2}{\mathcal{N}} \geq \sum_{z\in S_2(x)} d_z^- = \sum_{y\in S_1(x)} d_y^+$$

$$= \sum_{y\in S_1(x)} d_y - d_x - 2\#_\Delta(x). \tag{3.5}$$

Rearranging gives (3.3) as required. □

Definition 3.2 (The constant $\mathcal{K}_\infty^0(x)$)**.** Let $G = (V, E)$ be a locally finite simple graph. For any vertex $x \in V$, we define

$$\mathcal{K}_\infty^0(x) := 2 + \frac{d_x - av_1(x)}{2} + \frac{1}{2d_x} \sum_{y\in S_1(x)} \#_\Delta(x, y). \tag{3.6}$$

By the calculations in (3.5), we can reformulate $\mathcal{K}_\infty^0(x)$ as follows:

$$\mathcal{K}_\infty^0(x) = \frac{3 + d_x - av_1^+(x)}{2}. \tag{3.7}$$

In terms of the above definition, we can rewrite (3.3) as

$$\mathcal{K}_{G,x}(\mathcal{N}) \leq \mathcal{K}_\infty^0(x) - \frac{2d_x}{\mathcal{N}}.$$

Corollary 3.3. *Let $G = (V, E)$ be a d-regular graph and let $x \in V$. Then*

$$K_{G,x}(\infty) \leq 2 + \frac{\#_\Delta(x)}{d} = 2 + \frac{1}{2d} \sum_{y\in S_1(x)} \#_\Delta(x, y). \tag{3.8}$$

Proof. Follows immediately from Theorem 3.1 from noting that in a regular graph we have $d_x = av_1(x)$. □

Remark 3.4. We remark that on a d-regular graph, Klartag, Kozma, Ralli, and Tetali [21, Theorem 1.2] have derived an upper bound of $\mathcal{K}_{G,x}(\infty)$, via a different calculating method from here. Namely, they proved

$$\mathcal{K}_\infty(G, x) \leq 2 + \frac{1}{2} \max_{y\in S_1(x)} \#_\Delta(x, y). \tag{3.9}$$

We comment that their proof can also produce the stronger estimate (3.8).

Theorem 3.1 provides stronger estimates than Proposition 2.8. For example, we have the following one for regular graphs.

Corollary 3.5. *Let $G = (V, E)$ be a d-regular graph satisfying $CD(0, \mathcal{N})$. Then*

$$d \leq \frac{\mathcal{N} + \sqrt{\mathcal{N}^2 + 2\mathcal{N}\#_\Delta(x)}}{2}, \quad \text{for every } x \in V.$$

In particular, if G is triangle free, then $d \leq \mathcal{N}$.

Theorem 3.1 also tells cases that the curvature has to be negative. For example, we have the following straightforward consequence.

Corollary 3.6. *Let $G = (V, E)$ be a triangle free graph and let $x \in V$. Suppose that*

$$av_1(x) > 4 + d_x.$$

Then we have $\mathcal{K}_{G,x}(\infty) < 0$.

The local structures with negative curvature will be explored further in Section 6.

4. Fundamental properties of curvature functions

In this section, we discuss fundamental properties of the curvature function $\mathcal{K}_{G,x}$.

Proposition 4.1. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$. Then the curvature function $\mathcal{K}_{G,x} : (0, \infty] \to \mathbb{R}$ has the following properties:*

(i) *$\mathcal{K}_{G,x}$ is monotone non-decreasing.*
(ii) *$\mathcal{K}_{G,x}$ is continuous.*
(iii) *For any $\mathcal{N} \in (0, \infty]$, we have*

$$\mathcal{K}_{G,x}(\infty) - \frac{2d_x}{\mathcal{N}} \leq \mathcal{K}_{G,x}(\mathcal{N}) \leq \mathcal{K}^0_\infty(x) - \frac{2d_x}{\mathcal{N}}. \tag{4.1}$$

In particular, $\lim_{\mathcal{N}\to 0} \mathcal{K}_{G,x}(\mathcal{N}) = -\infty$.

(iv) *$\mathcal{K}_{G,x}$ is a concave function.*

Remarks 4.2. (i) Note that for a given vertex, $\mathcal{K}_{G,x}(\infty)$ and $\mathcal{K}^0_\infty(x)$ are both fixed constant. Hence, (4.1) describes a rough shape of the graph of the curvature function $\mathcal{K}_{G,x}$.
(ii) We are grateful to Bobo Hua and also to Jim Portegies, who independently raised the concavity question for this curvature function.

We first prove the following lemma.

Lemma 4.3. *For any $0 < \mathcal{N}_1 \leq \mathcal{N}_2 \leq \infty$, we have*

$$\mathcal{K}_{G,x}(\mathcal{N}_2) \leq \mathcal{K}_{G,x}(\mathcal{N}_1) + 2d_x \left(\frac{1}{\mathcal{N}_1} - \frac{1}{\mathcal{N}_2}\right) \tag{4.2}$$

Proof. By definition, we have

$$\begin{aligned} \Gamma_2(x) \geq& \frac{1}{\mathcal{N}_2}\Delta(x)^\top\Delta(x) + \mathcal{K}_{G,x}(\mathcal{N}_2)\Gamma(x) \\ =& \frac{1}{\mathcal{N}_1}\Delta(x)^\top\Delta(x) - \left(\frac{1}{\mathcal{N}_1} - \frac{1}{\mathcal{N}_2}\right)\Delta(x)^\top\Delta(x) + \mathcal{K}_{G,x}(\mathcal{N}_2)\Gamma(x). \end{aligned}$$

Observe that

$$d_x \cdot 2\Gamma - \Delta^\top\Delta = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & d_x I_{d_x} - J_{d_x} & \\ 0 & & & \end{pmatrix} \tag{4.3}$$

where I_{d_x} is the d_x by d_x identity matrix and J_{d_x} is the d_x by d_x matrix whose entries all equal 1. Since the matrix in (4.3) is diagonal dominant, we have

$$\Delta(x)^\top\Delta(x) \leq 2d_x\Gamma(x). \tag{4.4}$$

Inserting (4.4), we continue the calculation to obtain

$$\Gamma_2(x) \geq \frac{1}{\mathcal{N}_1}\Delta(x)^\top \Delta(x) + \left(\mathcal{K}_{G,x}(\mathcal{N}_2) - 2d_x\left(\frac{1}{\mathcal{N}_1} - \frac{1}{\mathcal{N}_2}\right)\right)\Gamma(x).$$

This implies (4.2). □

Now we are ready to show Proposition 4.1.

Proof of Proposition 4.1. (i). The monotonicity is clear from definition.

(ii). By (i) and Lemma 4.3, we have, for any $0 < \mathcal{N}_1 \leq \mathcal{N} \leq \infty$,

$$\mathcal{K}_{G,x}(\mathcal{N}_1) \leq \mathcal{K}_{G,x}(\mathcal{N}) \leq \mathcal{K}_{G,x}(\mathcal{N}_1) + 2d_x\left(\frac{1}{\mathcal{N}_1} - \frac{1}{\mathcal{N}}\right).$$

This shows $\mathcal{K}_{G,x} : (0,\infty] \to \mathbb{R}$ is a continuous function.

(iii). The upper bound in (4.1) is from Theorem 3.1 and the lower bound is from Lemma 4.3 by taking $\mathcal{N}_1 = \mathcal{N}$ and $\mathcal{N}_2 = \infty$.

(iv). Let $\mathcal{N}_1 < \mathcal{N}_2$ and $\mathcal{N} = \alpha\mathcal{N}_1 + (1-\alpha)\mathcal{N}_2$ for some $\alpha \in [0,1]$. Let $\mathcal{K}_j = \mathcal{K}_{G,x}(\mathcal{N}_j)$ for $j \in \{1,2\}$. We need to show that

$$\mathcal{K}_{G,x}(\mathcal{N}) \geq \alpha\mathcal{K}_1 + (1-\alpha)\mathcal{K}_2. \tag{4.5}$$

It follows from (1.2) that we have for any $f : V \to \mathbb{R}$, $j \in \{1,2\}$,

$$\mathcal{N}_j\Gamma_2(f)(x) - \mathcal{N}_j\mathcal{K}_j\Gamma(f)(x) \geq (\Delta f(x))^2.$$

This implies that

$$\mathcal{N}\Gamma_2(f)(x) - (\alpha\mathcal{N}_1\mathcal{K}_1 + (1-\alpha)\mathcal{N}_2\mathcal{K}_2)\,\Gamma(f)(x) \geq (\Delta f(x))^2. \tag{4.6}$$

Recall from the monotonicity of $\mathcal{K}_{G,x}$ that $\mathcal{K}_1 \leq \mathcal{K}_2$ and, therefore,

$$\alpha(1-\alpha)(\mathcal{N}_2 - \mathcal{N}_1)(\mathcal{K}_2 - \mathcal{K}_1) \geq 0.$$

This transforms straighforwardly into

$$\alpha\mathcal{N}_1\mathcal{K}_1 + (1-\alpha)\mathcal{N}_2\mathcal{K}_2 \geq (\alpha\mathcal{N}_1 + (1-\alpha)\mathcal{N}_2)\,(\alpha\mathcal{K}_1 + (1-\alpha)\mathcal{K}_2) = \mathcal{N}\,(\alpha\mathcal{K}_1 + (1-\alpha)\mathcal{K}_2)\,.$$

Plugging this into (4.6), using

$$\Gamma(f)(x) = \frac{1}{2}\sum_{y,y\sim x}(f(y) - f(x))^2 \geq 0,$$

and reversing the original calculations, we end up with

$$\Gamma_2(f)(x) \;\geq \frac{1}{\mathcal{N}}(\Delta f(x))^2 + (\alpha\mathcal{K}_1 + (1-\alpha)\mathcal{K}_2)\,\Gamma(f)(x).$$

This shows (4.5), finishing the proof. □

Proposition 4.1 (iii) implies that we can read the degree of x from its curvature function.

Corollary 4.4. *Let $G = (V,E)$ be a locally finite simple graph and $\mathcal{K}_{G,x} : (0,\infty] \to \mathbb{R}$ be the curvature function of $x \in V$. Then*

$$d_x = -\frac{1}{2}\lim_{\mathcal{N}\to 0}\mathcal{N}\mathcal{K}_{G,x}(\mathcal{N}).$$

The following property tells that, for any curvature function $\mathcal{K}_{G,x}$, there always exists a threshold $\mathcal{N}_0(x) \in (0,\infty]$ such that $\mathcal{K}_{G,x}$ is strictly monotone increasing on $(0,\mathcal{N}_0(x)]$, and is constant on $[\mathcal{N}_0(x),\infty]$.

Proposition 4.5. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$. If there exist $\mathcal{N}_1 < \mathcal{N}_2$ such that $\mathcal{K}_{G,x}(\mathcal{N}_1) = \mathcal{K}_{G,x}(\mathcal{N}_2)$, then we have*

$$\mathcal{K}_{G,x}(\mathcal{N}) = \mathcal{K}_{G,x}(\mathcal{N}_1) \quad \forall\, \mathcal{N} \in [\mathcal{N}_1, \infty]. \tag{4.7}$$

Proof. First, by monotonicity, we know $\mathcal{K}_{G,x}(\mathcal{N})$ is constant on $[\mathcal{N}_1, \mathcal{N}_2]$. Let us denote this constant by $K := \mathcal{K}_{G,x}(\mathcal{N}_1)$. Again, by monotonicity, we have $\mathcal{K}_{G,x}(\mathcal{N}) \geq K$ for all $\mathcal{N} \geq \mathcal{N}_2$. But the existence of $\mathcal{N} > \mathcal{N}_2$ with $\mathcal{K}_{G,x}(\mathcal{N}) > K$ would contradict to the concavity of $\mathcal{K}_{G,x}$ (w.r.t. the three points $\mathcal{N}_1 < \mathcal{N}_2 < \mathcal{N}$). This finishes the proof. □

Lemma 4.3 implies the following property on curvature sharpness.

Proposition 4.6. *Let $G = (V, E)$ be a locally finite graph and $x \in V$. If x is $\mathcal{N}$-curvature sharp, then x is $\mathcal{N}'$-curvature sharp for any $\mathcal{N}' \in (0, \mathcal{N}]$.*

Proof. If x is $\mathcal{N}$-curvature sharp, then $\mathcal{K}_{G,x}(\mathcal{N}) = \mathcal{K}^0_\infty(x) - 2d_x/\mathcal{N}$. By Lemma 4.3, we obtain, for any $\mathcal{N}' \in (0, \mathcal{N}]$,

$$\mathcal{K}_{G,x}(\mathcal{N}') \geq \mathcal{K}^0_\infty(x) - \frac{2d_x}{\mathcal{N}'}.$$

Recalling the upper bound in Theorem 3.1, we see the above equality holds. □

In particular, an ∞-curvature sharp vertex is $\mathcal{N}$-curvature sharp for any dimension $\mathcal{N} \in (0, \infty]$.

5. Reformulation of semidefinite programming problem and lower curvature bound

In this section, we derive a reformulation (see Theorem 5.4) of the semidefinite programming problem in Proposition 2.1. This leads to a lower bound of the curvature function $\mathcal{K}_{G,x}$ in terms of the upper bound $\mathcal{K}^0_\infty(x) - \frac{2d_x}{\mathcal{N}}$ and the minimal eigenvalue of a local matrix $\widehat{\mathcal{P}}_{\mathcal{N}}(x)$, which reflects the topological structure of the neighbourhood around x. When G is S_1-out regular at x, our lower bound estimate provides a precise formula for $\mathcal{K}_{G,x}$.

5.1. Main results without proofs.

We refer the readers for the proofs of the main results presented here to the next subsection.

Definition 5.1 (Matrices $\mathcal{P}_\infty$ and $\widehat{\mathcal{P}}_\infty$)**.** Let $G = (V, E)$ be a locally finite simple graph and let $x \in V$. $\widehat{\mathcal{P}}_\infty(x)$ is a $(d_x + 1)$ by $(d_x + 1)$ matrix defined as

$$\widehat{\mathcal{P}}_\infty(x) := \begin{pmatrix} 0 & d^+_{y_1} - av^+_1(x) & \cdots & d^+_{y_{d_x}} - av^+_1(x) \\ d^+_{y_1} - av^+_1(x) & & & \\ \vdots & & \mathcal{P}_\infty(x) & \\ d^+_{y_{d_x}} - av^+_1(x) & & & \end{pmatrix}, \tag{5.1}$$

where $\mathcal{P}_\infty(x)$ is a d_x by d_x matrix corresponding to the vertices in $S_1(x)$ given as follows. For any $i, j \in [d_x], i \neq j$, we have

$$(\mathcal{P}_\infty(x))_{ij} := 2 - 4w_{y_i y_j} - 4 \sum_{z \in S_2(x)} \frac{w_{y_i z} w_{z y_j}}{d^-_z}, \tag{5.2}$$

with w_{uv} as defined in (2.8) and, for any $i \in [d_x]$,

$$(\mathcal{P}_\infty(x))_{ii} := - \sum_{j \in [d_x], j \neq i} (\mathcal{P}_\infty)_{ij} - (d^+_{y_i} - av^+_1(x)). \tag{5.3}$$

Remark 5.2. Note that the entry $(\mathcal{P}_\infty(x))_{ij}$ in (5.2) is determined by the number of 1-paths between y_i and y_j (i.e., $w_{y_iy_j}$, which is either 0 or 1), and a weighted counting of the 2-paths between y_i and y_j via vertices in $S_2(x)$. The entry $(\mathcal{P}_\infty(x))_{ii}$ in (5.3) is defined such that

$$\widehat{\mathcal{P}}_\infty(x)\mathbf{1} = 0.$$

By a direct calculation, one can reformulate (5.3) as

$$(\mathcal{P}_\infty(x))_{ii} = -2(d_x - 1) + 3d^+_{y_i} + av^+_1(x) + 4d^0_{y_i} - 4\sum_{z\in S_2(x)} \frac{w^2_{y_iz}}{d^-_z}. \tag{5.4}$$

Definition 5.3 (Matrices $\widehat{\mathcal{P}}_\mathcal{N}$)**.** Let $G = (V,E)$ be a locally finite simple graph and let $x \in V$. For $\mathcal{N} \in (0,\infty]$, we define

$$\widehat{\mathcal{P}}_\mathcal{N}(x) := \widehat{\mathcal{P}}_\infty(x) + \frac{4}{\mathcal{N}}\begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & d_xI_{d_x} - J_{d_x} & \\ 0 & & & \end{pmatrix}. \tag{5.5}$$

By definition, we have $\widehat{\mathcal{P}}_\mathcal{N}\mathbf{1} = 0$.

Now, we are ready to state our main results.

Theorem 5.4. *Let $G = (V,E)$ be a locally finite simple graph and let $x \in V$. Then for any $\mathcal{N} \in (0,\infty]$, $\mathcal{K}_{G,x}(\mathcal{N})$ is the solution of the following semidefintie programming,*

$$\begin{aligned} &\textit{maximize } \mathcal{K}^0_\infty(x) - \frac{2d_x}{\mathcal{N}} - \frac{\lambda}{2} \\ &\textit{subject to } \widehat{\mathcal{P}}_\mathcal{N}(x) \geq -\lambda\cdot 2\Gamma(x). \end{aligned}$$

Moreover, the following are equivalent:

(i) $\mathcal{K}_{G,x}(\mathcal{N}) = \mathcal{K}^0_\infty(x) - \frac{2d_x}{\mathcal{N}} - \frac{\lambda}{2}$;

(ii) *The matrix $\widehat{\mathcal{P}}_\mathcal{N}(x) + \lambda\cdot 2\Gamma(x)$ is positive semidefinite and has zero eigenvalue of multiplicity at least 2.*

Theorem 5.4 can be considered as a new version of Proposition 2.1 and Corollary 2.7, in terms of the matrix $\widehat{\mathcal{P}}_\mathcal{N}(x) + \lambda\cdot 2\Gamma(x)$ instead of $4M_{K,\mathcal{N}}$. Note the latter matrix has a larger size.

As a consequence of Theorem 5.4, we have the following lower bound of the curvature function.

Theorem 5.5. *Let $G = (V,E)$ be a locally finite simple graph and let $x \in V$, Then for any $\mathcal{N} \in (0,\infty]$, we have*

$$\mathcal{K}_{G,x}(\mathcal{N}) \geq \mathcal{K}^0_\infty(x) - \frac{2d_x}{\mathcal{N}} + \frac{1}{2}\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x)). \tag{5.6}$$

The above estimate is sharp if and only if the zero eigenvalue of the matrix

$$\widehat{\mathcal{P}}_\mathcal{N}(x) - \lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))\cdot 2\Gamma(x)$$

has multiplicity at least 2.

Recall in Corollary 4.4 that we can read the degree d_x from the curvature function $\mathcal{K}_{G,x}$. With the help of Theorem 5.5, we can further read the average out degree $av^+_1(x)$.

Corollary 5.6. *Let $G=(V,E)$ be a locally finite simple graph and $\mathcal{K}_{G,x}:(0,\infty]\to\mathbb{R}$ be the curvature function of $x\in V$. Then*

$$av_1^+(x)=3+d_x-2\lim_{\mathcal{N}\to 0}\left(\mathcal{K}_{G,x}(\mathcal{N})+\frac{2d_x}{\mathcal{N}}\right).$$

Proof. Combining the upper bound in Theorem 3.1 and the lower bound in Theorem 5.5, we obtian

$$2\mathcal{K}_\infty^0(x)+\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))\le 2\left(\mathcal{K}_{G,x}(\mathcal{N})+\frac{2d_x}{\mathcal{N}}\right)\le 2\mathcal{K}_\infty^0(x)=3+d_x-av_1^+(x).$$

Therefore, it remains to prove $\lim_{\mathcal{N}\to 0}\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))=0$. Since $\widehat{\mathcal{P}}_\mathcal{N}(x)\mathbf{1}=0$, we only need to show for any $v=(v_0,v_1,\ldots,v_{d_x})^\top\in\mathbf{1}^\perp$, $\lim_{\mathcal{N}\to 0}v^\top\widehat{\mathcal{P}}_\mathcal{N}(x)v\ge 0$.

By (5.5), we calculate

$$\begin{aligned} v^\top\widehat{\mathcal{P}}_\mathcal{N}(x)v =& 2v_0\sum_{i=1}^{d}(d_{y_i}^+-av_1^+(x))v_i+\begin{pmatrix} v_1 & \cdots & v_{d_x}\end{pmatrix}\mathcal{P}_\infty\begin{pmatrix} v_1\\ \vdots \\ v_{d_x}\end{pmatrix}\\ &+\frac{4}{\mathcal{N}}\left[d_x\sum_{i=1}^{d_x}v_i^2-\left(\sum_{i=1}^{d_x}v_i\right)^2\right].\end{aligned}$$

If $v=(-d,1,\ldots,1)^\top$, we can check from above $v^\top\widehat{\mathcal{P}}_\mathcal{N}(x)v=0$. Otherwise, we have $d_x\sum_{i=1}^{d_x}v_i^2-\left(\sum_{i=1}^{d_x}v_i\right)^2>0$, and therefore $\lim_{\mathcal{N}\to 0}v^\top\widehat{\mathcal{P}}_\mathcal{N}(x)v=\infty$. □

When G is S_1-out regular at x, we obtain, from Theorem 5.5, a precise formula for calculating the curvature function $\mathcal{K}_{G,x}$. Note in this case, we have $\mathcal{P}_\infty(x)\mathbf{1}=0$, and, therefore, $\lambda_{\min}(\mathcal{P}_\infty(x))\le 0$.

Theorem 5.7. *Let $G=(V,E)$ be a locally finite simple graph and let $x\in V$. Assume that G is S_1-out regular at x, i.e.,*

$$d_{y_i}^+=av_1^+(x),\ \textit{for any } y_i\in S_1(x). \tag{5.7}$$

Then, we have for any $\mathcal{N}\in(0,\infty]$

$$\mathcal{K}_{G,x}(\mathcal{N})=\mathcal{K}_\infty^0(x)-\frac{2d_x}{\mathcal{N}}+\frac{1}{2}\lambda_{\min}\left(\mathcal{P}_\infty(x)+\frac{4}{\mathcal{N}}(d_xI_{d_x}-J_{d_x})\right). \tag{5.8}$$

More explicitly, we have

$$\mathcal{K}_{G,x}(\mathcal{N})=\begin{cases}\mathcal{K}_\infty^0(x)-\dfrac{2d_x}{\mathcal{N}}, & \textit{if } 0<\mathcal{N}\le\mathcal{N}_0(x);\\ \mathcal{K}_\infty^0(x)-\dfrac{2d_x}{\mathcal{N}_0(x)}, & \textit{if } \mathcal{N}>\mathcal{N}_0(x),\end{cases} \tag{5.9}$$

where

$$\mathcal{N}_0(x):=\frac{4d_x}{-\lambda_{\min}\left(\mathcal{P}_\infty(x)\right)}. \tag{5.10}$$

When $\lambda_{\min}\left(\mathcal{P}_\infty(x)\right)=0$, (5.10) reads as $\mathcal{N}_0(x)=\infty$.

Remark 5.8. When $d_x > 1$, $\mathbf{1}_{d_x}^{\perp} \neq \emptyset$, then $\mathcal{P}_\infty(x)\mathbf{1} = 0$ implies

$$\begin{aligned}\frac{1}{2}\lambda_{\min}\left(\mathcal{P}_\infty(x) + \frac{4}{\mathcal{N}}(d_x I_{d_x} - J_{d_x})\right) &= \min\left\{0, \frac{1}{2}\lambda_{\min}\left(\mathcal{P}_\infty(x)|_{\mathbf{1}^\perp}\right) + \frac{2}{\mathcal{N}}d_x\right\} \\ &= \begin{cases} 0, & \text{if } 0 < \mathcal{N} \leq \overline{\mathcal{N}}_0(x); \\ -\dfrac{2d_x}{\mathcal{N}_0(x)} + \dfrac{2d_x}{\mathcal{N}}, & \text{if } \mathcal{N} > \overline{\mathcal{N}}_0(x), \end{cases}\end{aligned}$$

where

$$\overline{\mathcal{N}}_0(x) := \begin{cases} \dfrac{4d_x}{-\lambda_{\min}\left(\mathcal{P}_\infty(x)|_{\mathbf{1}^\perp}\right)}, & \text{if } \lambda_{\min}\left(\mathcal{P}_\infty(x)|_{\mathbf{1}^\perp}\right) < 0; \\ \infty, & \text{if } \lambda_{\min}\left(\mathcal{P}_\infty(x)|_{\mathbf{1}^\perp}\right) \geq 0. \end{cases}$$

Since $\lambda_{\min}(\mathcal{P}_\infty(x)) = \min\{0, \lambda_{\min}\left(\mathcal{P}_\infty(x)|_{\mathbf{1}^\perp}\right)\}$, we have $\mathcal{N}_0(x) = \overline{\mathcal{N}}_0(x)$. Therefore (5.9) is a reformulation of (5.8). When $d_x = 1$, we observe $\mathcal{P}_\infty(x)$ and $d_x I_{d_x} - J_{d_x}$ are both one by one zero matrices, and, therefore, (5.9) coincides with (5.8).

Example 5.9 (Leaves)**.** Let $G = (V, E)$ be a locally finite simple graph. Let $x \in V$ be a leaf of G, i.e., $d_x = 1$. Then, since both $\mathcal{P}_\infty(x)$ and $d_x I_{d_x} - J_{d_x}$ are one by one zero matrices, we have for any $\mathcal{N} \in (0, \infty]$,

$$\mathcal{K}_{G,x}(\mathcal{N}) = 2 - \frac{av_1^+(x)}{2} - \frac{2}{\mathcal{N}}. \tag{5.11}$$

Theorem 5.7 tells that, when G is S_1-out regular at x, there always exists $\mathcal{N}_0(x) \in (0, \infty]$, such that x is $\mathcal{N}$-curvature sharp for any $\mathcal{N} \in (0, \mathcal{N}_0(x)]$, and $\mathcal{K}_{G,x}(\mathcal{N}) = \mathcal{K}_{G,x}(\mathcal{N}_0(x))$ is constant for $\mathcal{N} \in [\mathcal{N}_0(x), \infty]$. In fact, this property is a characterization of the S_1-out regularity of x.

Corollary 5.10. *Let $G = (V, E)$ be a locally finite simple graph. Then G is S_1-out regular at x if and only if there exists $\mathcal{N} \in (0, \infty]$ such that x is $\mathcal{N}$-curvature sharp.*

Proof. Assume that x is $\mathcal{N}$-curvature sharp for $\mathcal{N} \in (0, \infty]$. Then we obtain, by Theorem 5.4, $\widehat{\mathcal{P}}_{\mathcal{N}}(x) \geq 0$. Therefore, by Sylvester's criterion, we have for any $y_i \in S_1(x)$,

$$\det\begin{pmatrix} 0 & d_{y_i}^+ - av_1^+(x) \\ d_{y_i}^+ - av_1^+(x) & \mathcal{P}_\infty(x)_{ii} + \frac{4d_x}{\mathcal{N}} - 1 \end{pmatrix} = -(d_{y_i}^+ - av_1^+(x))^2 \geq 0.$$

This implies $d_{y_i}^+ = av_1^+(x)$ for any $y_i \in S_1(x)$.

The other direction is a straightforward consequence of Theorem 5.7. □

Corollary 5.10 and Theorem 5.7 implies the following characterization.

Corollary 5.11. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$. Then x is ∞-curvature sharp if and only if G is S_1-out regular at x and the matrix $\mathcal{P}_\infty(x) \geq 0$.*

In the following example, which will play an important role in Example 9.12, we illustrate how the above results can be applied to calculate explicit curvature functions.

Example 5.12. Figure 4 shows a 4-regular graph $G = (V, E)$ with two types of vertices, denoted by x_1, x_2, x_3 and y_1, y_2, y_3, y_4. We will now calculate the curvature functions $\mathcal{K}_{G,x_i}$ and $\mathcal{K}_{G,y_j}$ explicitly. The symmetries of the graph imply that these functions do not depend on i or j and it suffices to calculate $\mathcal{K}_{G,x_1}$ and $\mathcal{K}_{G,y_1}$.

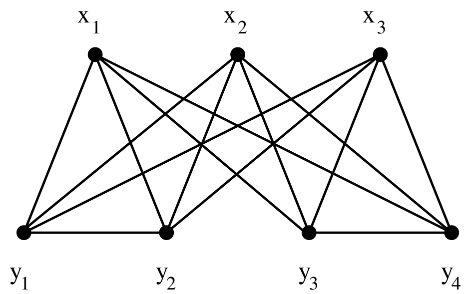

FIGURE 4. A 4-regular graph with two types of vertices x_i and y_j

For the calculation of $\mathcal{K}_{G,x_1}$, we observe that x_1 is S_1-out regular and apply Theorem 5.7. We have $av_1^+(x_1) = 2$ and (3.7) yields $\mathcal{K}_\infty^0(x_1) = \frac{5}{2}$. The matrix $\mathcal{P}_\infty(x_1)$ takes the simple form

$$\mathcal{P}_\infty(x_1) = \begin{pmatrix} 4 & -4 & 0 & 0 \\ -4 & 4 & 0 & 0 \\ 0 & 0 & 4 & -4 \\ 0 & 0 & -4 & 4 \end{pmatrix}$$

and has $\lambda_{\min}(\mathcal{P}_\infty(x_1)) = 0$ since it is diagonal dominant. Therefore $\mathcal{N}_0(x_1)$, defined in (5.10), is equal to infinity and we have

$$\mathcal{K}_{G,x_1}(\mathcal{N}) = \frac{5}{2} - \frac{8}{\mathcal{N}}.$$

The calculation of $\mathcal{K}_{G,y_1}$ is much more involved and, since y_1 is not S_1-out regular, we need to employ Theorem 5.4. From the structure of the punctured 2-ball $\mathring{B}_2(y_1)$ we can derive $av_1^+(y_1) = 3/2$ and $\mathcal{K}_\infty^0(y_1) = 11/4$. Therefore, we have

$$\mathcal{K}_{G,y_1}(\mathcal{N}) = \frac{11}{4} - \frac{8}{\mathcal{N}} - \frac{\lambda}{2}, \tag{5.12}$$

with $\lambda \geq 0$ chosen such that $\widehat{\mathcal{P}}_\mathcal{N}(y_1) + \lambda \cdot 2\Gamma(y_1)$ is positive semidefinite with zero eigenvalue of multiplicity at least 2. Recall that $\widehat{\mathcal{P}}_\mathcal{N}(y_1)$ was defined in (5.5) via $\widehat{\mathcal{P}}_\infty(y_1)$. $\widehat{\mathcal{P}}_\infty(y_1)$ and $2\Gamma(y_1)$, as matrices with entries corresponding to y_1, y_2, x_1, x_2, x_3, are given by

$$\widehat{\mathcal{P}}_\infty(y_1) = \begin{pmatrix} 0 & -\frac{3}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{3}{2} & \frac{15}{2} & -2 & -2 & -2 \\ \frac{1}{2} & -2 & \frac{17}{6} & -\frac{2}{3} & -\frac{2}{3} \\ \frac{1}{2} & -2 & -\frac{2}{3} & \frac{17}{6} & -\frac{2}{3} \\ \frac{1}{2} & -2 & -\frac{2}{3} & -\frac{2}{3} & \frac{17}{6} \end{pmatrix}, \quad \text{and } 2\Gamma(y_1) = \begin{pmatrix} 4 & -1 & -1 & -1 & -1 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

The eigenvalues of $\widehat{\mathcal{P}}_\mathcal{N}(y_1) + \lambda \cdot 2\Gamma(y_1)$ are 0, $(32 + 2\lambda\mathcal{N} + 7\mathcal{N})/(2\mathcal{N}) > 0$ with multiplicity 2, and

$$\frac{f(\lambda,\mathcal{N}) \pm \sqrt{f^2(\lambda,\mathcal{N}) + g(\lambda,\mathcal{N})}}{2\mathcal{N}}$$

with

$$f(\lambda,\mathcal{N}) = 6\mathcal{N}\lambda + 9\mathcal{N} + 16 > 0, \qquad \text{and } g(\lambda,\mathcal{N}) = 5\mathcal{N}(-4\mathcal{N}\lambda^2 - (36\mathcal{N} + 64)\lambda + 3\mathcal{N}).$$

For all eigenvalues to be non-negative and two of them to be 0, we need to have $g(\lambda, \mathcal{N}) = 0$, leading to

$$\lambda = \frac{-(9\mathcal{N} + 16) + \sqrt{3\mathcal{N}^2 + (9\mathcal{N} + 16)^2}}{2\mathcal{N}}.$$

Plugging this into (5.12), we obtain

$$\mathcal{K}_{G,y_1}(\mathcal{N}) = 5 - \frac{8 + \sqrt{21\mathcal{N}^2 + 72\mathcal{N} + 64}}{2\mathcal{N}}.$$

In particular, we have $\mathcal{K}_{G,x_i}(\infty) = 5/2$ for $i \in \{1,2,3\}$ and $\mathcal{K}_{G,y_j}(\infty) = 5 - \sqrt{21}/2 = 2.7087\ldots$ for $j \in \{1,2,3,4\}$.

Even though this can also be derived from the symmetries of the graph, the fact that the curvatures at x_i and y_j are different implies that there is no graph automorphism mapping a vertex x_i to a vertex y_j.

5.2. **Proofs of main results.** In the following, we prove Theorems 5.4, 5.5, and 5.7. Let us first show the following general result.

Proposition 5.13. *Let M be a symmetric square matrix such that*

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix},$$

where M_{11}, M_{22} are two square submatrices of orders m_1, m_2, respectively, and $M_{22} > 0$. Denote by $\mathcal{Q}(M)$ the matrix

$$\mathcal{Q}(M) := M_{11} - M_{12}M_{22}^{-1}M_{21}. \tag{5.13}$$

Then,

- (i) *$M \geq 0$ if and only if $\mathcal{Q}(M) \geq 0$;*
- (ii) *M has zero eigenvalue of multiplicity at least 2 if and only if $\mathcal{Q}(M)$ has zero eigenvalue of multiplicity at least 2.*
- (iii) *If $M\mathbf{1}_{m_1+m_2} = 0$, then $\mathcal{Q}(M)\mathbf{1}_{m_1} = 0$.*

Proof. Since $M_{22} > 0$, there exist a matrix $A_0 > 0$, such that $M_{22} = A_0 A_0^\top$. Set $C_0^\top := A_0^{-1}M_{21}$. Then we have $A_0 C_0^\top = M_{21}$, and

$$C_0 C_0^\top = M_{12}(A_0^{-1})^\top A_0^{-1} M_{21} = M_{12}M_{22}^{-1}M_{21}. \tag{5.14}$$

Therefore, we obtain

$$M = \begin{pmatrix} C_0 \\ A_0 \end{pmatrix} \begin{pmatrix} C_0^\top & A_0^\top \end{pmatrix} + \begin{pmatrix} \mathcal{Q}(M) & 0 \\ 0 & 0 \end{pmatrix}. \tag{5.15}$$

Observing the first matrix on the RHS of (5.15) is positive semidefinite, we conclude that $\mathcal{Q}(M) \geq 0$ implies $M \geq 0$.

Conversely, if $\mathcal{Q}(M) \ngeq 0$, then there exists a vector v, such that $v^\top \mathcal{Q}(M) v < 0$. Set

$$w := -(A_0^\top)^{-1} C_0^\top v. \tag{5.16}$$

We calculate

$$\begin{pmatrix} C_0^\top & A_0^\top \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix} = C_0^\top v + A_0^\top w = 0. \tag{5.17}$$

By (5.15), this implies

$$\begin{pmatrix} v^\top & w^\top \end{pmatrix} M \begin{pmatrix} v \\ w \end{pmatrix} = v^\top \mathcal{Q}(M) v < 0.$$

Hence, $M \not\geq 0$. This finishes the proof of (i).

Now we prove (ii). Let v_1, v_2 be two linearly independent eigenvectors of $\mathcal{Q}(M)$ corresponding to zero. We define the corresponding vectors $w_i, i = 1, 2$ via (5.16). Due to (5.17), we have

$$M \begin{pmatrix} v_i \\ w_i \end{pmatrix} = \mathcal{Q}(M) v_i = 0, \; i = 1, 2.$$

That is, we find two independent eigenvectors of M corresponding to eigenvalue zero.

Conversely, let $\begin{pmatrix} v_i \\ w_i \end{pmatrix}, i = 1, 2$ be two linearly independent eigenvectors of M corresponding to eigenvalue zero. We have

$$M \begin{pmatrix} v_i \\ w_i \end{pmatrix} = 0, \quad \text{implies} \quad \mathcal{Q}(M) v_i = 0, \tag{5.18}$$

by (5.15) and

$$\begin{pmatrix} C_0^\top & A_0^\top \end{pmatrix} \begin{pmatrix} v_i \\ w_i \end{pmatrix} = A_0^{-1} \begin{pmatrix} M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} v_i \\ w_i \end{pmatrix} = 0.$$

It remains to prove v_1 and v_2 are linearly independent. Suppose v_1 and v_2 are linearly dependent. W.o.l.g., we can assume $v_1 = v_2$. Then we get

$$M \begin{pmatrix} 0 \\ w_1 - w_2 \end{pmatrix} = 0, \text{ and, in particular, } \; M_{22}(w_1 - w_2) = 0.$$

Recall $M_{22} > 0$. We have $w_1 = w_2$. This contradicts to the fact that $\begin{pmatrix} v_i \\ w_i \end{pmatrix}, i = 1, 2$ are linearly independent. We now finish the proof of (ii).

(iii) is a particular case of (5.18). □

The following lemma is a key observation to apply Proposition 5.13 to our situation.

Lemma 5.14. *Let $G = (V, E)$ be a locally finite simple graph and let $x \in V$. Then we have*

$$\widehat{\mathcal{P}}_\infty(x) = (4\Gamma_2)_{B_1,B_1} - (4\Gamma_2)_{B_1,S_2} (4\Gamma_2)^{-1}_{S_2,S_2} (4\Gamma_2)_{S_2,B_1} - 2\mathcal{K}^0_\infty \cdot 2\Gamma. \tag{5.19}$$

Note we drop the dependence on x in the RHS of (5.19) for convenience.

Remark 5.15. Let us write

$$\Gamma_2 - \mathcal{K}^0_\infty \Gamma = \begin{pmatrix} (\Gamma_2)_{B_1,B_1} - \mathcal{K}^0_\infty \Gamma & (\Gamma_2)_{B_1,S_2} \\ (\Gamma_2)_{S_2,B_1} & (\Gamma_2)_{S_2,S_2} \end{pmatrix} \tag{5.20}$$

Then by (5.13), we can reformulate (5.19) as

$$\widehat{\mathcal{P}}_\infty = 4\mathcal{Q}(\Gamma_2 - \mathcal{K}^0_\infty \Gamma). \tag{5.21}$$

Proof. Recall (2.9), (2.10), and (2.11). We calculate

$$(4\Gamma_2)_{B_1,S_2}(4\Gamma_2)^{-1}_{S_2,S_2}(4\Gamma_2)_{S_2,B_1}$$

$$= \begin{pmatrix} d^-_{z_1} & \cdots & d^-_{z_{|S_2|}} \\ -2w_{y_1z_1} & \cdots & -2w_{y_1z_{|S_2|}} \\ \vdots & \vdots & \vdots \\ -2w_{y_{d_x}z_1} & \cdots & -2w_{y_{d_x}z_{|S_2|}} \end{pmatrix} \begin{pmatrix} \frac{1}{d^-_{z_1}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{1}{d^-_{z_{|S_2|}}} \end{pmatrix} \begin{pmatrix} d^-_{z_1} & \cdots & d^-_{z_{|S_2|}} \\ -2w_{y_1z_1} & \cdots & -2w_{y_1z_{|S_2|}} \\ \vdots & \vdots & \vdots \\ -2w_{y_{d_x}z_1} & \cdots & -2w_{y_{d_x}z_{|S_2|}} \end{pmatrix}^\top$$

$$(5.22)\quad = \begin{pmatrix} \sum_{z\in S_2} d^-_z & -2d^+_{y_1} & \cdots & -2d^+_{y_{d_x}} \\ -2d^+_{y_1} & 4\sum_{z\in S_2(x)} \frac{w^2_{y_1z}}{d^-_z} & \cdots & 4\sum_{z\in S_2(x)} \frac{w_{y_1z}w_{zy_{d_x}}}{d^-_z} \\ \vdots & \vdots & \ddots & \vdots \\ -2d^+_{y_{d_x}} & 4\sum_{z\in S_2(x)} \frac{w_{y_{d_x}z}w_{zy_1}}{d^-_z} & \cdots & 4\sum_{z\in S_2(x)} \frac{w^2_{y_{d_x}z}}{d^-_z} \end{pmatrix}.$$

On the other hand, using (2.2), (2.6), (2.7), and (3.7), we calculate

$$(4\Gamma_2)_{B_1,B_1} - 2\mathcal{K}^0_\infty \cdot 2\Gamma$$

$$(5.23)\quad = \begin{pmatrix} d_x\cdot av^+_1(x) & -d^+_{y_1} - av^+_1(x) & -d^+_{y_2} - av^+_1(x) & \cdots & -d^+_{y_{d_x}} - av^+_1(x) \\ -d^+_{y_1} - av^+_1(x) & (4\Gamma_2)_{y_1,y_1} - 2\mathcal{K}^0_\infty & 2-4w_{y_1y_2} & \cdots & 2-4w_{y_1y_{d_x}} \\ -d^+_{y_2} - av^+_1(x) & 2-4w_{y_2y_1} & (4\Gamma_2)_{y_2,y_2} - 2\mathcal{K}^0_\infty & \cdots & 2-4w_{y_2y_{d_x}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -d^+_{y_{d_x}} - av^+_1(x) & 2-4w_{y_{d_x}y_1} & 2-4w_{y_{d_x}y_2} & \cdots & (4\Gamma_2)_{y_{d_x},y_{d_x}} - 2\mathcal{K}^0_\infty \end{pmatrix},$$

where for any $y_i \in S_1$,

$$(4\Gamma_2)_{y_i,y_i} - 2\mathcal{K}^0_\infty = (5 - d_x + 3d^+_{y_i} + 4d^0_{y_i}) - (3 + d_x - av^+_1(x)) = -2(d_x-1) + 3d^+_{y_i} + av^+_1(x) + 4d^0_{y_i}.$$

Observe that

$$d_x \cdot av^+_1(x) = \sum_{y\in S_1(x)} d^+_y = \sum_{z\in S_2(x)} d^-_z.$$

Therefore, subtracting (5.22) from (5.23) produces the matrix $\widehat{\mathcal{P}}_\infty(x)$. □

Proof of Theorem 5.4. Recall Proposition 2.1: $\mathcal{K}_{G,x}(\mathcal{N})$ is the solution of the following semidefinite programming problem:

$$\text{maximize } K$$
$$\text{subject to } \Gamma_2(x) - \frac{1}{\mathcal{N}}\Delta(x)^\top\Delta(x) \geq K\Gamma(x).$$

We change the variable K in the above problem to λ, which is given by

$$(5.24)\qquad \lambda := 2\left(\mathcal{K}^0_\infty - \frac{2d_x}{\mathcal{N}} - K\right).$$

Let us write

$$M_{K,\mathcal{N}} := \Gamma_2 - \frac{1}{\mathcal{N}}\Delta^\top\Delta - K\Gamma = \begin{pmatrix} (\Gamma_2)_{B_1,B_1} - \frac{1}{\mathcal{N}}\Delta^\top\Delta - K\Gamma & (\Gamma_2)_{B_1,S_2} \\ (\Gamma_2)_{S_2,B_1} & (\Gamma_2)_{S_2,S_2} \end{pmatrix}.$$

Recalling (5.13), we have

$$\begin{aligned}4\mathcal{Q}(M_{K,\mathcal{N}}) =&4\mathcal{Q}(\Gamma_2-\mathcal{K}_\infty^0\Gamma)+4(\mathcal{K}_\infty^0-K)\Gamma-\frac{4}{\mathcal{N}}\Delta^\top\Delta\\ =&\widehat{\mathcal{P}}_\infty+\frac{4}{\mathcal{N}}\left(d_x\cdot 2\Gamma-\Delta^\top\Delta\right)+\lambda\cdot 2\Gamma.\end{aligned}$$

In the second equality above, we used Lemma 5.14. Recalling (4.3), we have, by (5.5),

$$4\mathcal{Q}(M_{K,\mathcal{N}})=\widehat{\mathcal{P}}_\mathcal{N}+\lambda\cdot 2\Gamma. \tag{5.25}$$

Applying Proposition 5.13 (i), we have $M_{K,\mathcal{N}}\geq 0$ if and only if $4\mathcal{Q}(M_{K,\mathcal{N}})\geq 0$. Hence, (5.25) implies that the semidefinite programming problem is equivalent to the one in Theorem 5.4.

Using (5.24) and (5.25), the equivalence of (i) and (ii) in Theorem 5.4 is then a straightforward consequence of Corollary 2.7 and Proposition 5.13. □

We remark that, by (5.25), the fact $\widehat{\mathcal{P}}_\mathcal{N}\mathbf{1}=0$ can also be derived from $M_{K,\mathcal{N}}\mathbf{1}=0$ and Proposition 5.13.

Proof of Theorem 5.5. Applying Theorem 5.4, we only need to show

$$\widehat{\mathcal{P}}_\mathcal{N}(x)-\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))\cdot 2\Gamma(x)\geq 0. \tag{5.26}$$

Let us denote the above matrix by L for short. If $d_x=1$, we have $d_y^+=av_1^+(x)$ for the neighbor y of x. Recall $\widehat{\mathcal{P}}_\mathcal{N}(x)\mathbf{1}=0$. We have $\widehat{\mathcal{P}}_\mathcal{N}(x)\mathbf{1}$ is a zero matrix. Therefore, (5.26) is true. If $d_x>1$, (5.26) is true because $\widehat{\mathcal{P}}_\mathcal{N}(x)\mathbf{1}=0$, $2\Gamma(x)\mathbf{1}=0$, and

$$\begin{aligned}\lambda_{\min}(L|_{\mathbf{1}^\perp})\geq&\lambda_{\min}\left(\widehat{\mathcal{P}}_\mathcal{N}(x)\Big|_{\mathbf{1}^\perp}\right)-\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))\cdot\lambda_{\min}(2\Gamma(x)|_{\mathbf{1}^\perp})\\ =&\lambda_{\min}\left(\widehat{\mathcal{P}}_\mathcal{N}(x)\Big|_{\mathbf{1}^\perp}\right)-\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))\geq 0.\end{aligned}$$

In the first inequality above, we used the fact $\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N})\leq 0$, which follows from $\widehat{\mathcal{P}}_\mathcal{N}(x)\mathbf{1}=0$, and in the subsequent equality, we used Proposition 2.2. □

Proof of Theorem 5.7. Since $d_{y_i}^+=av_1^+(x)$ for any $y_i\in S_1(x)$, we have

$$\widehat{\mathcal{P}}_\mathcal{N}(x)=\begin{pmatrix}0 & 0 & \cdots & 0\\ 0 & & & \\ \vdots & & \mathcal{P}_\infty(x)+\frac{4}{\mathcal{N}}(d_xI_{d_x}-J_{d_x}) & \\ 0 & & & \end{pmatrix}. \tag{5.27}$$

Hence $\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))=\lambda_{\min}\left(\mathcal{P}_\infty(x)+\frac{4}{\mathcal{N}}(d_xI_{d_x}-J_{d_x})\right)$. If $\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))=0$, then the equality (5.8) follows from Theorem 5.5 and the upper bound in Theorem 3.1.

Otherwise, we have $\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))<0$. By Theorem 5.5, it remains to show the matrix

$$\widehat{\mathcal{P}}_\mathcal{N}(x)-\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N})(x)\cdot 2\Gamma(x) \tag{5.28}$$

has at least two independent zero eigenvectors. Recall the constant vector $\mathbf{1}_{d_x+1}$ is one zero eigenvector. Since $\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N}(x))<0$, there exist $v=(v_0,v_1,\ldots,v_{d_x})\in\mathbf{1}_{d_x+1}^\perp$ which is the eigenvector of $\widehat{\mathcal{P}}_N$ corresponding to $\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N})$. By (5.27), we can assume $v_0=0$. Then we check $2\Gamma v=v$. (Recall Proposition 2.2). Therefore, v is another zero eigenvector of $\widehat{\mathcal{P}}_\mathcal{N}-\lambda_{\min}(\widehat{\mathcal{P}}_\mathcal{N})\cdot 2\Gamma$. □

5.3. **Families of examples.** We now employ our results to discuss several families of examples.

Example 5.16 (Regular trees)**.** Let $T_d = (V, E)$ be a d-regular tree and $x \in V$. We have

$$\mathcal{K}_{T_d,x}(\mathcal{N}) = \begin{cases} 2 - \dfrac{2d}{\mathcal{N}}, & \text{if } 0 < \mathcal{N} \leq 2; \\ 2 - d, & \text{if } \mathcal{N} > 2. \end{cases} \tag{5.29}$$

Proof. For any $y \in S_1(x)$, we have $d_y^+ = av_1^+(x) = d - 1$. Hence T_d is S_1-out regular at x and we apply Theorem 5.7. Note all the off-diagonal entries of $\mathcal{P}_\infty(x)$ equal 2. Then by the property $\mathcal{P}_\infty(x)\mathbf{1} = 0$, we obtain

$$\mathcal{P}_\infty(x) = -2(dI_d - J_d). \tag{5.30}$$

Observe that the set of eigenvalues of the matrix $dI_d - J_d$ is

$$\sigma(dI_d - J_d) = \{0, \underbrace{d, \ldots, d}_{d-1}\}. \tag{5.31}$$

Therefore, $\lambda_{\min}(\mathcal{P}_\infty(x)) = -2d$, and $\mathcal{N}_0(x)$, defined in (5.10), is 2. Noticing that

$$\mathcal{K}_\infty^0(x) = \frac{3 + d_x - av_1^+(x)}{2} = 2,$$

we obtain (5.29) from (5.9). □

While regular trees are $\mathcal{N}$-curvature sharp only for $\mathcal{N} \in (0, 2]$, we will see the complete graphs are curvature sharp for any $\mathcal{N} \in (0, \infty]$.

Example 5.17 (Complete graphs)**.** Let $K_n = (V, E)$ be the complete graph on $n \geq 2$ vertices and $x \in V$. For any $\mathcal{N} \in (0, \infty]$, we have

$$\mathcal{K}_{K_n,x}(\mathcal{N}) = \frac{n+2}{2} - \frac{2(n-1)}{\mathcal{N}}. \tag{5.32}$$

We remark that (5.32) has been obtained in [20, Proposition 3] via different calculating method. Below we show (5.32) follows immediately from Theorem 5.7.

Proof. We check $d_x = n - 1$ and $d_y^+ = av_1^+(x) = 0$, for any $y \in S_1(x)$. Therefore,

$$\mathcal{K}_\infty^0(x) = \frac{3 + d_x - av_1^+(x)}{2} = \frac{n+2}{2}. \tag{5.33}$$

Since $w_{y_i y_j} = 1$ for any pair of vertices in $S_1(x)$, all off-diagonal entries of $\mathcal{P}_\infty(x)$ equal -2. By the property $\mathcal{P}_\infty(x)\mathbf{1} = 0$, we know

$$P_\infty(x) = 2(n-1)I_{n-1} - 2J_{n-1}. \tag{5.34}$$

Recall (5.31), we have $\lambda_{\min}(\mathcal{P}_\infty(x)) = 0$. Hence, we have $\mathcal{N}_0(x)$, defined in (5.10), equal ∞. By (5.9), we obtain (5.32). □

Next, we consider the family of complete bipartite graphs, which are possibly irregular, but are still S_1-out regular.

Example 5.18 (Complete bipartite graphs)**.** Let $K_{m,n} = (V, E)$ be a complete bipartite graph. Let $x \in V$ be a vertex with degree $d_x = n$. If $n = 1$ or $n \leq 2m-2$, we have for any $\mathcal{N} \in (0, \infty]$

$$\mathcal{K}_{K_{m,n},x}(\mathcal{N}) = \frac{4+n-m}{2} - \frac{2n}{\mathcal{N}}. \tag{5.35}$$

If, otherwise, $n \neq 1$ and $n > 2m-2$, we have

$$\mathcal{K}_{K_{m,n},x}(\mathcal{N}) = \begin{cases} \dfrac{4+n-m}{2} - \dfrac{2n}{\mathcal{N}}, & \text{if } 0 < \mathcal{N} \leq \frac{2n}{n-2m+2}; \\ \dfrac{3m-n}{2}, & \text{if } \mathcal{N} > \frac{2n}{n-2m+2}. \end{cases} \tag{5.36}$$

In particular, we have $\mathcal{K}_{K_{1,1}}(\infty) = 2$ and, when $(n, m) \neq (1, 1)$,

$$\mathcal{K}_{K_{m,n},x}(\infty) = \frac{m+2-|n-2m+2|}{2}. \tag{5.37}$$

Remark 5.19. We remark that $K_{2,6}$ has constant flat curvature, i.e., $\mathcal{K}_{K_{2,6},x}(\infty) = 0\ \forall x$. But at each vertex x with degree 2, $\mathcal{K}_{K_{2,6},x}(\mathcal{N}) < 0$ for any finite dimension $\mathcal{N}$. This has already been observed in Example 2.13. On the other hand, at each vertex y with degree 6, we see $\mathcal{K}_{K_{2,6},y}(\mathcal{N}) = 0$, for any $\mathcal{N} \in [3, \infty]$.

Proof. Let $x \in V$ be a vertex such that $d_x = n$. Then, we have $d_y^+ = av_1^+(x) = m-1, d_y^0 = 0$, for any $y \in S_1(x)$. Therefore, we obtain

$$\mathcal{K}_\infty^0(x) = \frac{3+d_x-av_1^+(x)}{2} = \frac{4+n-m}{2}. \tag{5.38}$$

Note that $d_z^- = n$, for any $y \in S_1(x)$, and there are $(m-1)$ 2-paths connecting any two vertices $y_i, y_j \in S_1(x)$ via a vertex in $S_2(x)$. Therefore, each off-diagonal entry of $\mathcal{P}_\infty(x)$ equals $2 - \frac{4}{n}(m-1)$. By the property that $\mathcal{P}_\infty(x)\mathbf{1} = 0$, we have

$$\mathcal{P}_\infty(x) = -\frac{2}{n}(n-2m+2)(nI_n - J_n).$$

Recalling (5.31), we have $\sigma(\mathcal{P}_\infty(x)) = \{0, -2(n-2m+2), \ldots, -2(n-2m+2)\}$.

If $n = 1$ or $n \leq 2m-2$, i.e., if $n = m = 1$ or $n \leq 2m-2$, we have $\lambda_{\min}(\mathcal{P}_\infty(x)) = 0$. Hence, $\mathcal{N}_0(x) = \infty$. We obtain (5.35) by (5.9). If, otherwise, $n \neq 1$ and $n > 2m-2$, we have $\lambda_{\min}(\mathcal{P}_\infty(x)) = -2(n-2m+2)$. Hence, $\mathcal{N}_0(x) = \frac{2n}{n-2m+2}$. Noticing that

$$\mathcal{K}_\infty^0(x) - \frac{2d_x}{\mathcal{N}_0(x)} = \frac{4+n-m}{2} - (n-2m-2) = \frac{3m-n}{2},$$

we obtain (5.36) by (5.9). □

Particularly, we have the curvature function for star graphs $Star_n = K_{1,n}$. We can suppose $n \geq 2$. (Recall when $n = 1$, $Star_1 = K_{1,1} = K_2$.)

From the above examples, we can derive the curvature function for cycles.

Example 5.20 (Cycles)**.** Let $C_n = (V, E)$ be a cycle graph with n vertices and $x \in V$. Since $C_3 = K_3$, we have, by Example 5.17, for any $\mathcal{N} \in (0, \infty]$,

$$\mathcal{K}_{C_3,x}(\mathcal{N}) = \frac{5}{2} - \frac{4}{\mathcal{N}}. \tag{5.39}$$

Since $C_4 = K_{2,2}$, we have, by Example 5.18, for any $\mathcal{N} \in (0, \infty]$,

$$\mathcal{K}_{C_4,x}(\mathcal{N}) = 2 - \frac{4}{\mathcal{N}}. \tag{5.40}$$

When $n \geq 5$, the local subgraph $B_2(x)$ is isomorphic to that of a vertex in a 2-regular tree (i.e., infinite path). Therefore, we have, by Example 5.16,

$$\mathcal{K}_{C_n,x}(\mathcal{N}) = \begin{cases} 2 - \dfrac{4}{\mathcal{N}}, & \text{if } 0 < \mathcal{N} \leq 2; \\ 0, & \text{if } \mathcal{N} > 2, \end{cases} \quad \text{for} \quad n \geq 5. \tag{5.41}$$

6. Curvature and connectedness of $\mathring{B}_2(x)$

In this section, we prove relations between the curvature function $\mathcal{K}_{G,x}$ at a vertex $x \in V$ and topological properties of the punctured 2-ball $\mathring{B}_2(x)$. More precisely, we show that

- **(a):** The curvature $\mathcal{K}_{G,x}(\infty)$ is – with very few exceptions – always negative if $\mathring{B}_2(x)$ consists of more than one connected component.
- **(b):** The curvature function $\mathcal{K}_{G,x}$ does not decrease under adding edges in $S_1(x)$, or merging two vertices in $S_2(x)$ which do not have common neighbours. Obviously, these operation increases the connectedness of $\mathring{B}_2(x)$.

6.1. **Connected components and negative curvature.** Let $G = (V, E)$ be a locally finite simple graph, $x \in V$ be a vertex and $d = d_x$ its degree. Henceforth we assume that we have chosen a specific connected component of $\mathring{B}_2(x)$. We denote the vertices of this connected component in $S_1(x)$ and $S_2(x)$ by $y_1, \ldots, y_r$ and $z_1, \ldots, z_s$, respectively. Figure 5 illustrates connected components of $\mathring{B}_2(x)$. Note that the punctured 2-ball $\mathring{B}_2(x)$ has more than one component if and only if $d > r$.

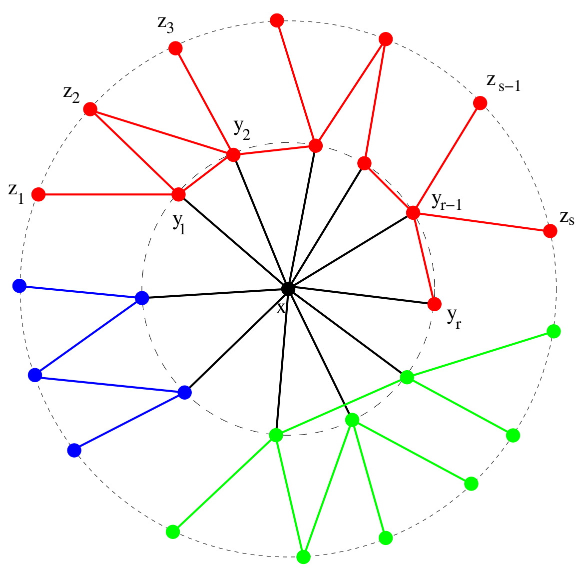

Figure 5. Connected components of $\mathring{B}_2(x)$ in different colours; choosing the red connected component leads to $d = 11$ and $r = 6$.

Our first two results assume that $\mathring{B}_2(x)$ has more than one connected component and distinguish the cases $s > 0$ (our connected component has vertices in $S_2(x)$) and $s = 0$ (our connected component consists entirely of vertices in $S_1(x)$). Our first result deals with the case that our connected component of $\mathring{B}_2(x)$ has only vertices in $S_1(x)$.

Lemma 6.1. *Assume that $\mathring{B}_2(x)$ has more than one connected component (i.e., $d > r$) and that $s = 0$ and $d \geq 4$. Then we have $\mathcal{K}_{G,x}(\infty) < 0$.*

For the proofs, it is useful to introduce the notions $\mathbf{0}_t$ and $\mathbf{1}_t$ for the all-zero and the all-one column vector of size t.

Proof. Let A be the submatrix of $4\Gamma_2(x)$ corresponding to the vertices x, $y_1, \ldots, y_r$. Let C be the $(2 \times (r+1))$ matrix

$$C = \begin{pmatrix} 1 & \mathbf{0}_r^\top \\ 0 & \mathbf{1}_r^\top \end{pmatrix}.$$

Then the (2×2) matrix $A_0 = CAC^\top$ has the form

$$A_0 = \begin{pmatrix} 3d + d^2 & -r(3+d) \\ -r(3+d) & r(5-d) + 2r(r-1) \end{pmatrix}.$$

Since

$$\det A_0 = -(3+d)r(d-3)(d-r), \tag{6.1}$$

$d \geq 4$ implies $\det A_0 < 0$ and A_0 cannot be positive semidefinite. This implies $\mathcal{K}_{G,x}(\infty) < 0$. □

Our second result reads as follows.

Lemma 6.2. *Assume that $\mathring{B}_2(x)$ has more than one connected component (i.e., $d > r$) and that $s > 0$ and $d \geq 3$. Then we have $\mathcal{K}_{G,x}(\infty) < 0$.*

Proof. Let A be the submatrix of $4\Gamma_2(x)$ corresponding to the vertices x, $y_1, \ldots, y_r$, $z_1, \ldots, z_s$. Let C be the $(3 \times (1+r+s))$ matrix

$$C = \begin{pmatrix} 1 & \mathbf{0}_r^\top & \mathbf{0}_s^\top \\ 0 & \mathbf{1}_r^\top & \mathbf{0}_s^\top \\ 0 & \mathbf{0}_r^\top & \mathbf{1}_s^\top \end{pmatrix}.$$

Then the (3×3) matrix $A_0 = CAC^\top$ has the form

$$A_0 = \begin{pmatrix} 3d + d^2 & -(3+d)r - S & S \\ -(3+d)r - S & r(5-d) + 3S + 2r(r-1) & -2S \\ S & -2S & S \end{pmatrix} \tag{6.2}$$

with $S = \sum_{i=1}^r d_{y_i}^{out} = \sum_{j=1}^s d_{z_j}^{in} \geq s$. Choosing the row vector $v = (r, d, d + 1/S)$, we obtain

$$v^\top A_0 v = -rd(d-3)(d-r) - 2(d-r) + \frac{1}{S} \leq \frac{1}{S} - 2(d-r) \leq \frac{1}{S} - 4 \leq -3 < 0. \tag{6.3}$$

This shows that A is not positive semidefinite and, therefore, $\mathcal{K}_{G,x}(\infty) < 0$. □

In the situation described in Lemma 6.2, we can only have $\mathcal{K}_{G,x}(\infty) > 0$ if $d = 2$ and, consequently, $r = 1$. In this case, there is only one vertex of our connected component, denoted by y, in $S_1(x)$, and the next result tells us that $\mathcal{K}_{G,x}(\infty) < 0$ unless the out degree of y satisfies $d_y^+ = 1$.

Lemma 6.3. *Assume that $d = 2$ and $\mathring{B}_2(x)$ has two connected components, i.e., $S_1(x) = \{y, y'\}$ and $y \not\sim y'$. Then we have $\mathcal{K}_{G,x}(\infty) < 0$ if $d_y^+ \geq 2$ or $d_{y'}^+ \geq 2$.*

Proof. Following the proof of Lemma 6.2, we are in the special case $(d, r) = (2, 1)$ and $S = d_y^+$. The matrix A_0 from (6.2) then simplifies to

$$A_0 = \begin{pmatrix} 10 & -(5+S) & S \\ -(5+S) & 3+3S & -2S \\ S & -2S & S \end{pmatrix},$$

and we have $\det A_0 = S(5-3S)$. If $d_y^+ = S \geq 2$, we obtain $\det A_0 < 0$, i.e., $4\Gamma_0$ cannot be positive semidefinite and we have $\mathcal{K}_{G,x}(\infty) < 0$. The same holds true when we replace y by y', finishing the proof. □

Theorem 6.4. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$. If $\mathring{B}_2(x)$ has more than one connected component then $\mathcal{K}_{G,x}(\infty) < 0$, except for one of the five cases (a)-(e) presented in Figure 6.*

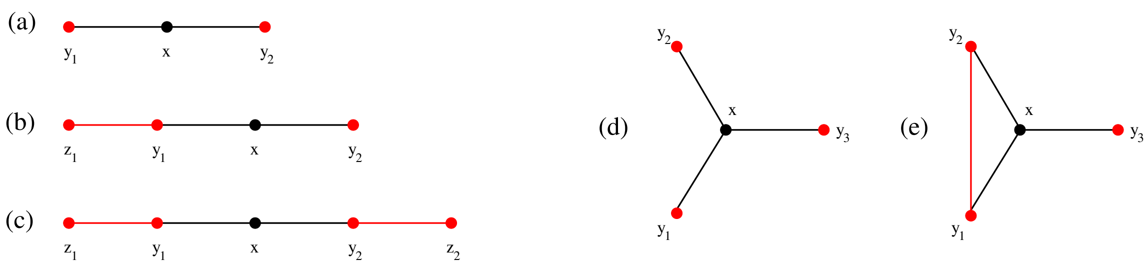

FIGURE 6. 2-balls $B_2(x)$ with $\mathcal{K}_{G,x}(\infty) \geq 0$. The corresponding punctured 2-balls $\mathring{B}_2(x)$ are red.

Proof. We assume that $\mathring{B}_2(x)$ has at least two connected components and, therefore, $d \geq 2$. If $d \geq 4$ we have $\mathcal{K}_{G,x}(\infty) < 0$ by Lemmata 6.1 and 6.2. So it only remains to investigate $2 \leq d \leq 3$.

If $S_2(x) \neq \emptyset$, there exists a connected component of $\mathring{B}_2(x)$ with a vertex in $S_2(x)$ and Lemma 6.2 implies $\mathcal{K}_{G,x}(\infty) < 0$ if $d = 3$. So we are left with $d = 2$ and, in view of Lemma 6.3, the only remaining possibilities for $B_2(x)$ to achieve $\mathcal{K}_{G,x}(\infty) \geq 0$ in the case $S_2(x) \neq \emptyset$ are (b) or (c).

In the case $S_2(x) = \emptyset$, $d = 2$ and $\mathcal{K}_{G,x}(\infty) \geq 0$ lead necessarily to the configuration (a) for $B_2(x)$. Similarly, $d = 3$ and $\mathcal{K}_{G,x}(\infty) \geq 0$ lead necessarily to the configurations (d) and (e). □

Theorem 6.4 and the curvature calculations for the exceptional cases have the following immediate consequences.

Definition 6.5. Let $G = (V, E)$ be be a locally finite simple graph. An edge $e \in E$ is called an (r, s)-*bridge* if the graph G decomposes after removal of the edge $e = \{x, y\}$ into two separate non-empty components and if the degrees of the vertices x and y in each of the components after removal of e are r and s, respectively.

Corollary 6.6. *Let $G = (V, E)$ be be a locally finite simple graph and $e = \{x, y\} \in E$ be an (r, s)-bridge.*

(a) *If $r = 0$, x is a leaf and the curvature function $\mathcal{K}_{G,x}$ is given by*

$$\mathcal{K}_{G,x}(\mathcal{N}) = 2 - \frac{s}{2} - \frac{2}{\mathcal{N}}.$$

In particular, we have $\mathcal{K}_{G,x}(\infty) \geq 0$ iff $s \leq 4$.

(b) *If* $r = 1$*, we can only have* $\mathcal{K}_{G,x}(\infty) \geq 0$ *if* $s \in \{0, 1\}$.
(c) *If* $r = 2$*, we have* $\mathcal{K}_{G,x}(\infty) \leq 0$*, and we can only have equality if* $s = 0$.
(d) *If* $r \geq 3$*, we have always* $\mathcal{K}_{G,x}(\infty) < 0$.

Proof. The case $r = 0$ follows from Example 5.9. In all other cases, $\mathring{B}_2(x)$ has at least two connected components and we can directly apply Theorem 6.4. □

Definition 6.7. Let $G = (V, E)$ be be a locally finite simple graph and $e \in E$. The *girth of* e, denoted by $\mathrm{girth}(e)$ is the length of the shortest circuit in G containing e. If e is not contained in any circuit, we define $\mathrm{girth}(e) = \infty$.

Corollary 6.8. *Let* $G = (V, E)$ *be be a locally finite simple graph and* $e = \{x, y\} \in E$*. If* $5 \leq \mathrm{girth}(e) < \infty$*, we have* $\mathcal{K}_{G,x}(\infty), \mathcal{K}_{G,y}(\infty) \leq 0$.

If $\mathrm{girth}(e) = \infty$*, the only exceptions for* $\mathcal{K}_{G,x}(\infty) < 0$ *are: (i)* $d_x \geq 2$ *and we have one of the situations (a)-(e) in Figure 6 for* $B_2(x)$*, (ii)* x *is a leaf and the other vertex has degree* ≤ 5.

Proof. The girth condition $5 \leq \mathrm{girth}(e) < \infty$ implies that $\mathring{B}_2(x)$ has at least two connected components and we can apply Theorem 6.4. So we only have to consider the exceptional cases. The exceptional cases (a) and (b) imply $\mathrm{girth}(e) = \infty$, and we have in the cases (c), (d), (e) that $\mathcal{K}_{G,x}(\infty) = 0$. The same holds true for the vertex y.

Now we assume $\mathrm{girth}(e) = \infty$. If $d_x \geq 2$, $\mathring{B}_2(x)$ must have at least two connected components and we can apply Theorem 6.4. The only exceptions of $\mathcal{K}_{G,x}(\infty) < 0$ are then situations (a)-(e) in Figure 6. If $d_x = 1$, we know from Example 5.9 that it has only non-negative curvature if the degree of its neighbour is ≤ 5, which is precisely the case (ii). □

Remark 6.9. In [19], B. Hua and Y. Lin classified graphs with girth at least 5 and satisfying $CD(0, \infty)$. Their work was carried out independently, provides related but different results, and considers, in contrast to our context, the normalized case.

6.2. **Operations that do not decrease the curvature.** In this subsection, we discuss operations that does not decrease the curvature. The first one is adding new spherical edges in $S_1(x)$.

Proposition 6.10. *Let* $G = (V, E)$ *be a graph and* $x \in V$ *be a vertex. Let* $G' = (V, E')$ *be the graph obtained from* G *by adding a new spherical edge in* $S_1(x)$*. Then we have for any* $\mathcal{N} \in (0, \infty]$,

$$\mathcal{K}(G', x; \mathcal{N}) \geq \mathcal{K}(G, x; \mathcal{N}).$$

Proof. Suppose that G' is obtained from G by adding a new edge $\{y_1, y_2\}$, where $y_1, y_2 \in S_1(x)$. Then we have

$$\Delta'(x) = \Delta(x), \ \Gamma'(x) = \Gamma(x),$$

and

$$\Gamma_2'(x) - \Gamma_2(x) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & (\Gamma_2)'_{S_1,S_1} - (\Gamma_2)_{S_1,S_1} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

By (2.7), we obtain that

$$(\Gamma_2)'_{S_1,S_1} - (\Gamma_2)_{S_1,S_1} = \begin{pmatrix} 1 & -1 & \cdots & 0 \\ -1 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}, \tag{6.4}$$

is positive semidefinite. This completes the proof. □

Remark 6.11. By Corollary 2.7, $\mathcal{K}(G', x; \mathcal{N}) = \mathcal{K}(G, x; \mathcal{N})$ if and only if the multiplicity of zero eigenvalue of $\Gamma_2'(x) - \frac{1}{\mathcal{N}}\Delta'(x)^\top\Delta'(x) - \mathcal{K}(G, x; \mathcal{N})\Gamma'(x)$ is no smaller than 2.

Merging two vertices z_1, z_2 in $S_2(x)$ also does not decrease the curvature. Here we assume the two vertices z_1, z_2 do not have common neighbours. By merging two vertices z_1, z_2, we mean the following operations: Remove the possible edge connecting z_1 and z_2 and identify z_1, z_2 as a new vertex z, where edges incident to z each correspond to an edge incident to either z_1 or z_2. The assumption that z_1, z_2 do not have common neighbours ensures that no multi-edge is produced by this operation.

Proposition 6.12. *Let $G = (V, E)$ be a graph and $x \in V$ be a vertex. Let $G'' = (V'', E'')$ be the graph obtained from G by merging two vertices in $S_2(x)$ which do not have common neighbours. Then we have for any $\mathcal{N} \in (0, \infty]$,*

$$\mathcal{K}(G'', x; \mathcal{N}) \geq \mathcal{K}(G, x; \mathcal{N}).$$

Proof. Suppose that G'' is obtained from G by merging the two vertices $z_{|S_2(x)|-1}, z_{|S_2(x)|}$ in $S_2(x)$ which do not have common neighbours. Then we have $\Delta''(x) = \Delta(x)$, $\Gamma''(x) = \Gamma(x)$. Let C'' be a $|B_2(x)| - 1$ by $|B_2(x)|$ matrix

$$C'' = \begin{pmatrix} I_{|B_2(x)|-2} & \mathbf{0}_{|B_2(x)|-2} & \mathbf{0}_{|B_2(x)|-2} \\ \mathbf{0}_{|B_2(x)|-2}^\top & 1 & 1 \end{pmatrix}.$$

Then we have

$$\Gamma_2''(x) = C''\Gamma_2(x)(C'')^\top.$$

Therefore, we have

$$\begin{aligned} &\Gamma_2''(x) - \frac{1}{\mathcal{N}}(\Delta''(x))^\top\Delta''(x) - \mathcal{K}(G, x, \mathcal{N})\Gamma''(x) \\ =&C''(\Gamma_2(x) - \frac{1}{\mathcal{N}}\Delta(x)^\top\Delta(x) - \mathcal{K}(G, x, \mathcal{N})\Gamma(x))(C'')^\top \geq 0. \end{aligned}$$

This finishes the proof. □

We believe the following property is true.

Conjecture 6.13. Let $G = (V, E)$ be a graph and $x \in V$ be a vertex. Let $G''' = (V''', E''')$ be the graph obtained from G by one of the following two operations:

- Delete a leaf in $S_2(x)$ and its incident edge.
- Delete $z \in S_2(x)$ and its incident edges $\{\{y, z\} \in E : y \in S_1(x)\}$; Adding an new edge between every two of $\{y \in S_1(x) : \{y, z\} \in E\}$.

Then we have for any $\mathcal{N} \in (0, \infty]$,

$$\mathcal{K}(G''', x; \mathcal{N}) \geq \mathcal{K}(G, x; \mathcal{N}).$$

7. Curvature functions of Cartesian products

In this section, we show that the curvature functions of a Cartesian product can be explicitly determined from curvature functions of the factors.

7.1. $*$**-product of functions.** We first discuss an abstract product between functions. Let us denote by $\mathcal{FK}$ the set of continuous, monotone non-decreasing functions $f : (0, \infty] \to \mathbb{R}$ with

$$\lim_{\mathcal{N} \to 0} f(\mathcal{N}) = -\infty.$$

Recalling Proposition 4.1, curvature functions lie in $\mathcal{FK}$.

For any $\mathcal{N} \in (0, \infty)$, let $D_k(\mathcal{N})$ be the following set:

$$D_k(\mathcal{N}) := \{(\mathcal{N}_1, \ldots, \mathcal{N}_k) : \mathcal{N}_j > 0 \ \text{ for all } \ j \text{ and } \mathcal{N}_1 + \cdots + \mathcal{N}_k = \mathcal{N}.\}. \tag{7.1}$$

Definition 7.1 ($*$-product)**.** For two functions $f_1, f_2 \in \mathcal{FK}$, we define $f_1 * f_2 : (0, \infty] \to \mathbb{R}$ as follows. For any $\mathcal{N} \in (0, \infty)$, let

$$f_1 * f_2(\mathcal{N}) := f_1(\mathcal{N}_1) = f_2(\mathcal{N}_2), \tag{7.2}$$

where $(\mathcal{N}_1, \mathcal{N}_2) \in D_2(\mathcal{N})$ is chosen such that

$$f_1(\mathcal{N}_1) = f_2(\mathcal{N}_2). \tag{7.3}$$

For $\mathcal{N} = \infty$, we define

$$f_1 * f_2(\infty) := \lim_{\mathcal{N} \to \infty} f_1 * f_2(\mathcal{N}). \tag{7.4}$$

Remark 7.2. Let us first verify that the $*$*-product is well defined.*

For two functions $f_1, f_2 \in \mathcal{FK}$ and $\mathcal{N} \in (0, \infty)$, there always exists a pair $(\mathcal{N}_1, \mathcal{N}_2) \in D_2(\mathcal{N})$ satisfying (7.3): We assume $f_1(\mathcal{N}/2) \le f_2(\mathcal{N}/2)$ without loss of generality (otherwise, we interchange the functions). By the Intermediate Value Theorem, the monotonicity of f_1, and $\lim_{h \to \mathcal{N}/2} f_2(\mathcal{N}/2 - h) = -\infty$, we can find $0 < h < \mathcal{N}/2$ such that

$$f_1(\mathcal{N}_1 + h) = f_2(\mathcal{N}_2 - h).$$

Note that $(\mathcal{N}_1 + h, \mathcal{N}_2 - h) \in D_2(\mathcal{N})$ is then the required pair.

Secondly, if there exist two pairs $(\mathcal{N}_1, \mathcal{N}_2), (\mathcal{N}_1', \mathcal{N}_2') \in D_2(\mathcal{N})$ such that (7.3) holds, then we have

$$f_1(\mathcal{N}_1) = f_1(\mathcal{N}_1') \text{ and } f_2(\mathcal{N}_2) = f_2(\mathcal{N}_2'). \tag{7.5}$$

Due to the definition of $D_2(\mathcal{N})$, we can choose i, j such that $\{i, j\} = \{1, 2\}$ and $\mathcal{N}_i \le \mathcal{N}_i'$, $\mathcal{N}_j \ge \mathcal{N}_j'$. Then (7.5) follows from the monotonicity of f_1 and f_2.

Thirdly, the limit $\lim_{\mathcal{N} \to \infty} f_1 * f_2(\mathcal{N})$ exists. For any $0 < \mathcal{N}_1 \le \mathcal{N}_2 < \infty$, Let $(\mathcal{N}_{11}, \mathcal{N}_{12}) \in D_2(\mathcal{N}_1), (\mathcal{N}_{21}, \mathcal{N}_{22}) \in D_2(\mathcal{N}_2)$ be two tuples such that

$$f_1 * f_2(\mathcal{N}_i) = f_1(\mathcal{N}_{i1}) = f_2(\mathcal{N}_{i2}), \ \ i = 1, 2.$$

Since there always exists $j \in \{1, 2\}$ with $\mathcal{N}_{1j} \le \mathcal{N}_{2j}$, we have, from the monotonicity of f_j,

$$f_1 * f_2(\mathcal{N}_1) = f_j(\mathcal{N}_{1j}) \le f_j(\mathcal{N}_{2j}) = f_1 * f_2(\mathcal{N}_2) \le f_j(\infty).$$

That is, $f_1 * f_2$ is a monotone non-decreasing function, bounded above by $f_j(\infty) < \infty$. Therefore, the limit exists.

We have the following equivalent definition of the $*$-product.

Proposition 7.3. *Let $f_1, f_2 \in \mathcal{FK}$ and $F : (0, \infty] \to \mathbb{R}$. Then $F = f_1 * f_2$ if and only if we have, for any $\mathcal{N}_1, \mathcal{N}_2 \in (0, \infty)$,*

$$\min\{f_1(\mathcal{N}_1), f_2(\mathcal{N}_2)\} \le F(\mathcal{N}_1 + \mathcal{N}_2) \le \max\{f_1(\mathcal{N}_1), f_2(\mathcal{N}_2)\}, \tag{7.6}$$

and $F(\infty) = \lim_{\mathcal{N} \to \infty} F(\mathcal{N})$.

Proof. If $F = f_1 * f_2$, there exists a tuple $(\mathcal{N}_1', \mathcal{N}_2') \in D_2(\mathcal{N}_1 + \mathcal{N}_2)$ such that

$$F(\mathcal{N}_1 + \mathcal{N}_2) = f_1(\mathcal{N}_1') = f_2(\mathcal{N}_2').$$

Recall there always exist $\{i, j\} = \{1, 2\}$ such that $\mathcal{N}_i \le \mathcal{N}_i'$ and $\mathcal{N}_j \ge \mathcal{N}_j'$. Then we obtain (7.6) by the monotonicity of f_1, f_2. $F(\infty) = \lim_{\mathcal{N}\to\infty} F(\mathcal{N})$ follows directly from Definition 7.1.

Let $F : (0, \infty] \to \mathbb{R}$ be a function satisfying (7.6) and $F(\infty) = \lim_{\mathcal{N}\to\infty} F(\mathcal{N})$. By Remark 7.2, for any $\mathcal{N} \in (0, \infty)$, there exists a pair $(\mathcal{N}_1, \mathcal{N}_2) \in D_2(\mathcal{N})$, such that

$$f(\mathcal{N}_1) = f_2(\mathcal{N}_2).$$

Therefore, (7.6) implies $F(\mathcal{N}) = f_1 * f_2(\mathcal{N})$, finishing the proof. □

Corollary 7.4. *Let $f_1, f_2 \in \mathcal{FK}$. Then for $\mathcal{N} \in (0, \infty)$, we have*

$$f_1 * f_2(\mathcal{N}) \le \min\{f_1(\mathcal{N}), f_2(\mathcal{N})\}. \tag{7.7}$$

For $\mathcal{N} = \infty$, we have

$$f_1 * f_2(\infty) = \min\{f_1(\infty), f_2(\infty)\}. \tag{7.8}$$

Proof. For $\mathcal{N} \in (0, \infty)$, assume $f_1(\mathcal{N}) \le f_2(\mathcal{N})$ without loss of generality. Note from the definition of the $*$-product that there exists $\mathcal{N}_1 \in (0, N]$ with

$$f_1 * f_2(\mathcal{N}) = f_1(\mathcal{N}_1).$$

Using monotonicity of f_1, we conclude that

$$f_1 * f_2(\mathcal{N}) \le f_1(\mathcal{N}) = \min\{f_1(\mathcal{N}), f_2(\mathcal{N})\},$$

proving (7.7). Furthermore, we have, by (7.6) and (7.7),

$$\min\{f_1(\mathcal{N}/2), f_2(\mathcal{N}/2)\} \le f_1 * f_2(\mathcal{N}) \le \min\{f_1(\mathcal{N}), f_2(\mathcal{N})\}.$$

Letting $\mathcal{N} \to \infty$, we prove (7.8). □

We further have the following basic properties of the $*$-product.

Proposition 7.5. *Let $f_1, f_2 \in \mathcal{FK}$. Then we have the following properties:*

(i) *(Commutativity)* $f_1 * f_2 = f_2 * f_1$.
(ii) *(Closedness)* $f_1 * f_2 \in \mathcal{FK}$.

Proof. (i) is obvious from the definition.

For (ii), recall first that we have shown monotonicity of $f_1 * f_2$ in Remark 7.2.

For any $\mathcal{N} \in (0, \infty)$, let $(\mathcal{N}_1, \mathcal{N}_2) \in D_2(\mathcal{N})$ be the pair with

$$f_1 * f_2(\mathcal{N}) = f_1(\mathcal{N}_1) = f_2(\mathcal{N}_2).$$

Then by monotonicity of f_2 and Proposition 7.3, we have for any $\epsilon > 0$,

$$f_2(\mathcal{N}_2) \le f_1 * f_2(\mathcal{N} + \epsilon) \le f_2(\mathcal{N}_2 + \epsilon).$$

By continuity of f_2, we see $f_1 * f_2$ is continuous at $\mathcal{N}$. Since by definition, $f_1 * f_2(\infty) := \lim_{\mathcal{N}\to\infty} f_1 * f_2(\mathcal{N})$, we prove that $f_1 * f_2 : (0, \infty] \to \mathbb{R}$ is continuous.

The property $\lim_{\mathcal{N}\to 0} f_1 * f_2(\mathcal{N}) = -\infty$ follows directly from Proposition 7.3 and $\lim_{\mathcal{N}\to 0} f_i(\mathcal{N}) = -\infty$, $i = 1, 2$. This finishes the proof of $f_1 * f_2 \in \mathcal{FK}$. □

The following proposition shows associativity of the $*$-product and implies, therefore, the well-definedness of k-fold products.

Proposition 7.6. *For $f_1, f_2, f_3 \in \mathcal{FK}$, we have associativity*

$$(f_1 * f_2) * f_3 = f_1 * (f_2 * f_3).$$

For functions $f_1, \ldots, f_k \in \mathcal{FK}$, $k \geq 2$, and $\mathcal{N} \in (0, \infty)$, we have

$$f_1 * \cdots * f_k(\mathcal{N}) = f_1(\mathcal{N}_1) = \cdots f_k(\mathcal{N}_k),$$

for any tuple $(\mathcal{N}_1, \ldots, \mathcal{N}_k) \in D_k(\mathcal{N})$ with

$$f_1(\mathcal{N}_1) = \cdots = f_k(\mathcal{N}_k).$$

Moreover, such a tuple always exists. For $\mathcal{N} = \infty$, we have

$$f_1 * \cdots * f_k(\infty) = \min\{f_1(\infty), \cdots, f_k(\infty)\}. \tag{7.9}$$

In particular, we have

$$\underbrace{f * \cdots * f}_{k}(\mathcal{N}) = f(\mathcal{N}/k), \quad \forall\, \mathcal{N} \in (0, \infty]. \tag{7.10}$$

Proof. Let $f_1, f_2, f_3 \in \mathcal{FK}$ and $\mathcal{N} \in (0, \infty)$. The expressions $(f_1 * f_2) * f_3$ and $f_1 * (f_2 * f_3)$ are well-defined due to closedness of $*$.

We show first the following fact for $\mathcal{N}_1, \mathcal{N}_2, \mathcal{N}_3, \mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3 > 0$: If

$$\mathcal{N}_1 + \mathcal{N}_2 + \mathcal{N}_3 = \mathcal{M}_1 + \mathcal{M}_2 + \mathcal{M}_3, \quad f_1(\mathcal{N}_1) = f_2(\mathcal{N}_2) = f_3(\mathcal{N}_3) \quad \text{and} \quad f_1(\mathcal{M}_1) = f_2(\mathcal{M}_2) = f_3(\mathcal{M}_3),$$

then $f_1(\mathcal{N}_1) = f_1(\mathcal{M}_1)$: Obviously, we can find $i, j \in \{1, 2, 3\}$ such that $\mathcal{N}_i \geq \mathcal{M}_i$ and $\mathcal{N}_j \leq \mathcal{M}_j$ and, using the monotonicity of the functions f_k,

$$f_1(\mathcal{N}_1) = f_i(\mathcal{N}_i) \geq f_i(\mathcal{M}_i) = f_1(\mathcal{M}_1) = f_j(\mathcal{M}_j) \geq f_j(\mathcal{N}_j) = f_1(\mathcal{N}_1),$$

which shows $f_1(\mathcal{N}_1) = f_1(\mathcal{M}_1)$.

Next we show that, for every $\mathcal{N} \in (0, \infty)$, there exist $\mathcal{N}_1, \mathcal{N}_2, \mathcal{N}_3 > 0$ with $\mathcal{N}_1 + \mathcal{N}_2 + \mathcal{N}_3 = \mathcal{N}$ and

$$(f_1 * f_2) * f_3(\mathcal{N}) = f_1(\mathcal{N}_1) = f_2(\mathcal{N}_2) = f_3(\mathcal{N}_3).$$

By Definition 7.1, we have $\mathcal{N}_1', \mathcal{N}_3 > 0$ with $\mathcal{N}_1' + \mathcal{N}_3 = \mathcal{N}$ such that

$$(f_1 * f_2) * f_3(\mathcal{N}) = f_1 * f_2(\mathcal{N}_1') = f_3(\mathcal{N}_3).$$

Applying Definition 7.1 again, we find $\mathcal{N}_1, \mathcal{N}_2 > 0$ with $\mathcal{N}_1 + \mathcal{N}_2 = \mathcal{N}_1'$ such that

$$f_1 * f_2(\mathcal{N}_1') = f_1(\mathcal{N}_1) = f_2(\mathcal{N}_2).$$

Combining these facts, we obtain

$$(f_1 * f_2) * f_3(\mathcal{N}) = f_1(\mathcal{N}_1) = f_2(\mathcal{N}_2) = f_3(\mathcal{N}_3)$$

with $\mathcal{N}_1 + \mathcal{N}_2 + \mathcal{N}_3 = \mathcal{N}$ as claimed.

Analogously, one can show that there are $\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3 > 0$ satisfying $\mathcal{M}_1 + \mathcal{M}_2 + \mathcal{M}_3 = \mathcal{N}$ and

$$f_1 * (f_2 * f_3)(\mathcal{N}) = f_1(\mathcal{M}_1) = f_2(\mathcal{M}_2) = f_3(\mathcal{M}_3).$$

Now, our first fact implies that

$$(f_1 * f_2) * f_3(\mathcal{N}) = f_1(\mathcal{N}_1) = f_1(\mathcal{M}_1) = f_1 * (f_2 * f_3)(\mathcal{N}),$$

which shows associativity for finite arguments $\mathcal{N} > 0$.

The same arguments lead to the statement about the $*$-product of k functions $f_1, \ldots, f_k \in \mathcal{FK}$ for arguments $\mathcal{N} \in (0, \infty)$ in the proposition. Associativity and the statements about $*$-products of k functions for the argument $\mathcal{N} = \infty$ in the proposition are easy applications of (7.8).

Finally, (7.10) can be shown by taking the tuple $(\mathcal{N}/k, \ldots, \mathcal{N}/k) \in D_k(\mathcal{N})$ when $\mathcal{N} \in (0, \infty)$, and by using (7.9) when $\mathcal{N} = \infty$. □

Proposition 7.7. *Let $f_1, f_2, g \in \mathcal{FK}$. The following are equivalent:*

(i) $f_1 * g \neq f_2 * g$.

(ii) *There exist $\mathcal{N}_0 \in (0, \infty]$ such that $f_1(\mathcal{N}_0) \neq f_2(\mathcal{N}_0)$ and $f_1(\mathcal{N}_0), f_2(\mathcal{N}_0) \leq g(\infty)$.*

Proof. (ii) ⇒ (i). W.l.o.g., we can suppose $f_1(\mathcal{N}_0) < f_2(\mathcal{N}_0)$. We can further suppose

$$f_2(\mathcal{N}_0) < g(\infty).$$

This is because, if $f_2(\mathcal{N}_0) = g(\infty)$, we can choose an $\mathcal{N}_0' < \mathcal{N}_0$, such that $f_2(\mathcal{N}_0') \in (f_1(\mathcal{N}_0), g(\infty))$. Then we have $f_1(\mathcal{N}_0') \leq f_1(\mathcal{N}_0) < f_2(\mathcal{N}_0') < g(\infty)$.

When $\mathcal{N}_0 \in (0, \infty)$, let $\mathcal{M}_0 = \min\{\mathcal{M}' \in (0, \infty) : g(\mathcal{M}') = f_2(\mathcal{N}_0)\}$. Then we have

$$f_2 * g(\mathcal{N}_0 + \mathcal{M}_0) = f_2(\mathcal{N}_0) = g(\mathcal{M}_0).$$

By assumption, we know $f_1(\mathcal{N}_0) < g(\mathcal{M}_0)$. Hence, there exists $\epsilon > 0$ such that

$$f_1 * g(\mathcal{N}_0 + \mathcal{M}_0) = f_1(\mathcal{N}_0 + \epsilon) = g(\mathcal{M}_0 - \epsilon).$$

By the choice of M_0, we have

$$f_1 * g(\mathcal{N}_0 + \mathcal{M}_0) = g(\mathcal{M}_0 - \epsilon) < g(\mathcal{M}_0) = f_2 * g(\mathcal{N}_0 + \mathcal{M}_0).$$

When $\mathcal{N}_0 = \infty$, we have, by Corollary 7.4,

$$f_1 * g(\infty) = f_1(\infty) < f_2(\infty) = f_2 * g(\infty).$$

This finishes the proof of (i) assuming (ii).

(i) ⇒ (ii). We prove this by showing its contrapositive. Suppose, for any $\mathcal{N} \in (0, \infty]$, we have

$$f_1(\mathcal{N}) = f_2(\mathcal{N}) \text{ or } \max\{f_1(\mathcal{N}), f_2(\mathcal{N})\} > g(\infty). \tag{7.11}$$

For any $\mathcal{N} \in (0, \infty)$, there exists $\mathcal{M}_1, \mathcal{M}_2 \in (0, \mathcal{N})$ such that

$$f_i * g(\mathcal{N}) = f_i(\mathcal{M}_i) = g(\mathcal{N} - \mathcal{M}_i), \ i = 1, 2.$$

If $\mathcal{M}_1 = \mathcal{M}_2$, then $f_1 * g(\mathcal{N}) = f_2 * g(\mathcal{N})$. Otherwise, we suppose $\mathcal{M}_1 < \mathcal{M}_2$ without loss of generality. By monotonicity, we have

$$f_1(\mathcal{M}_1) = g(\mathcal{N} - \mathcal{M}_1) \geq g(\mathcal{N} - \mathcal{M}_2) = f_2(\mathcal{M}_2).$$

This implies $g(\infty) \geq f_1(\mathcal{M}_1) \geq f_2(\mathcal{M}_2) \geq f_2(\mathcal{M}_1)$. By (7.11), we have $f_1(\mathcal{M}_1) = f_2(\mathcal{M}_1) = f_2(\mathcal{M}_2)$ and therefore, $f_1 * g(\mathcal{N}) = f_2 * g(\mathcal{N})$.

Letting $\mathcal{N} \to \infty$, we obtain $f_1 * g(\infty) = f_2 * g(\infty)$. This finishes the proof. □

Example 7.8. Given $a \in \mathbb{R}, b_1, b_2 \in (0, \infty)$, let $f_1, f_2 \in FK$ be the following two functions:

$$f_1(\mathcal{N}) := a - \frac{b_1}{\mathcal{N}} \text{ and } f_2(\mathcal{N}) := a - \frac{b_2}{\mathcal{N}}.$$

Then we have

$$f_1 * f_2(\mathcal{N}) = a - \frac{b_1 + b_2}{\mathcal{N}}, \ \forall\, \mathcal{N} \in (0, \infty]. \tag{7.12}$$

This can be verified by taking the tuple $\left(\frac{b_1}{b_1+b_2}\mathcal{N}, \frac{b_2}{b_1+2}\mathcal{N}\right) \in D_2(\mathcal{N})$ when $\mathcal{N} \in (0, \infty)$.

7.2. **Main results.** Given two locally finite simple graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, their Cartesian product $G_1 \times G_2 = (V_1 \times V_2, E_{12})$ is a locally finite graph with vertex set $V_1 \times V_2$ and edge set E_{12} given by the following rule. Two vertices $(x_1, y_1), (x_2, y_2) \in V_1 \times V_2$ are connected by an edge in E_{12} if

$$x_1 = x_2, \{y_1, y_2\} \in E_2 \quad \text{or} \quad \{x_1, x_2\} \in E_1, y_1 = y_2.$$

We have the following result.

Theorem 7.9. *Let $G_i = (V_i, E_i), i = 1, 2$ be two locally finite simple graphs. Then for any $x \in V_1$ and $y \in V_2$, we have*

$$\mathcal{K}_{G_1 \times G_2,(x,y)} = \mathcal{K}_{G_1,x} * \mathcal{K}_{G_2,y}. \tag{7.13}$$

Theorem 7.9 is derived from the following two Theorems, using Proposition 7.3, .

Theorem 7.10 ([28])**.** *Let $G_i = (V_i, E_i), i = 1, 2$ be two locally finite simple graphs. Then we have, for any $x \in V_1, y \in V_2$ and $\mathcal{N}_1, \mathcal{N}_2 \in (0, \infty]$,*

$$\mathcal{K}_{G_1 \times G_2,(x,y)}(\mathcal{N}_1 + \mathcal{N}_2) \geq \min\{\mathcal{K}_{G_1,x}(\mathcal{N}_1), \mathcal{K}_{G_2,y}(\mathcal{N}_2)\}. \tag{7.14}$$

Theorem 7.10 has been shown in [28, Theorem 2.5]. In this section, we further prove the following estimate.

Theorem 7.11. *Let $G_i = (V_i, E_i), i = 1, 2$ be two locally finite simple graphs. Then we have, for any $x \in V_1, y \in V_2$ and $\mathcal{N}_1, \mathcal{N}_2 \in (0, \infty]$,*

$$\mathcal{K}_{G_1 \times G_2,(x,y)}(\mathcal{N}_1 + \mathcal{N}_2) \leq \max\{\mathcal{K}_{G_1,x}(\mathcal{N}_1), \mathcal{K}_{G_2,y}(\mathcal{N}_2)\}. \tag{7.15}$$

We first recall a technical lemma from [28, Lemma 2.6]. Let $F : V_1 \times V_2 \to \mathbb{R}$ be a function on the product graph. For fixed $y \in V_2$, we will write $F_y(\cdot) := F(\cdot, y)$ as a function on V_1. Similarly, $F^x(\cdot) := F(x, \cdot)$. It is straightforward to check

$$\Delta F(x, y) = \Delta F_y(x) + \Delta F^x(y) \quad \text{and} \quad \Gamma(F)(x, y) = \Gamma(F_y)(x) + \Gamma(F^x)(y). \tag{7.16}$$

Lemma 7.12 ([28])**.** *For any function $F : V_1 \times V_2 \to \mathbb{R}$ and any $(x, y) \in V_1 \times V_2$, we have*

$$\begin{aligned}\Gamma_2(F)(x, y) =& \Gamma_2(F_y)(x) + \Gamma_2(F^x)(y) \\ &+ \frac{1}{2} \sum_{x_i \sim x} \sum_{y_k \sim y} \left(F(x_i, y_k) - F(x, y_k) - F(x_i, y) + F(x, y)\right)^2.\end{aligned} \tag{7.17}$$

where the operators Γ_2 are understood to be on different graphs according to the functions they are acting on.

Proof of Theorem 7.11. Let $f_1 : V_1 \to \mathbb{R}$ be a function with $\Gamma(f_1)(x) \neq 0$, such that

$$\Gamma_2(f_1)(x) = \frac{1}{\mathcal{N}_1}(\Delta f_1(x))^2 + \mathcal{K}_{G_1,x}(\mathcal{N}_1)\Gamma(f_1)(x). \tag{7.18}$$

Let $f_2 : V_2 \to \mathbb{R}$ be a function with $\Gamma(f_2)(x) \neq 0$, such that

$$\Gamma_2(f_2)(x) = \frac{1}{\mathcal{N}_2}(\Delta f_2(x))^2 + \mathcal{K}_{G_2,x}(\mathcal{N}_2)\Gamma(f_2)(x). \tag{7.19}$$

Let c_1, c_2 be two nonnegative real number. We define a function $F : V_1 \times V_2 \to \mathbb{R}$ such that

$$F_y(\cdot) := c_1 f_1(\cdot) + c_2 f_2(y), \quad F^x(\cdot) := c_2 f_2(\cdot) + c_1 f_1(x), \tag{7.20}$$

and, for any $\{x_i, x\} \in E_1$ and any $\{y_k, y\} \in E_2$,

$$F(x_i, y_k) := c_1 f_1(x_i) + c_2 f_2(y_k). \tag{7.21}$$

Then we obtain, from Lemma 7.12,

$$\Gamma_2(F)(x,y) = \Gamma_2(F_y)(x) + \Gamma_2(F^x)(y) = c_1^2\Gamma_2(f_1)(x) + c_2^2\Gamma_2(f_2)(y).$$

Inserting (7.18) and (7.19), we have

$$\begin{aligned}\Gamma_2(F)(x,y) = {}& \frac{1}{\mathcal{N}_1}\Delta(c_1 f_1(x))^2 + \frac{1}{\mathcal{N}_2}\Delta(c_2 f_2(y))^2 \\ & + \mathcal{K}_{G_1,x}(\mathcal{N}_1)\Gamma(c_1 f_1)(x) + \mathcal{K}_{G_1,y}(\mathcal{N}_2)\Gamma(c_2 f_2)(y).\end{aligned} \tag{7.22}$$

If $0 < \mathcal{N}_1, \mathcal{N}_2 < \infty$ and $\Delta f_1(x)$, $\Delta f_2(y)$ are not simultaneously zero, say $\Delta f_1(x) \neq 0$, we set

$$c_1 = \frac{\mathcal{N}_1^2 \Delta f_2(y)}{\mathcal{N}_2^2 \Delta f_1(x)}, \quad c_2 = 1.$$

Then we have

$$\frac{\mathcal{N}_2}{\mathcal{N}_1} c_1 \Delta f_1(x) = \frac{\mathcal{N}_1}{\mathcal{N}_2} c_2 \Delta f_2(y),$$

and hence

$$\frac{1}{\mathcal{N}_1}\Delta(c_1 f_1(x))^2 + \frac{1}{\mathcal{N}_2}\Delta(c_2 f_2(y))^2 = \frac{1}{\mathcal{N}_1 + \mathcal{N}_2}\left(c_1\Delta f_1(x) + c_2 \Delta f_2(x)\right)^2 \tag{7.23}$$

Using (7.16)and (7.23), we derive from (7.22)

$$\Gamma_2(F)(x,y) \leq \frac{1}{\mathcal{N}_1 + \mathcal{N}_2}\left(\Delta F(x,y)\right)^2 + \max\left\{\mathcal{K}_{G_1,x}(\mathcal{N}_1), \mathcal{K}_{G_1,y}(\mathcal{N}_2)\right\}\Gamma(F)(x,y). \tag{7.24}$$

This implies (7.15) in this case.

If, otherwise, $\Delta f_1(x) = \Delta f_2(y) = 0$ or at least one of $\mathcal{N}_1, \mathcal{N}_2$ equals ∞, say, $\mathcal{N}_1 = \infty$, we set

$$c_1 = 1, \quad c_2 = 0.$$

Then we show (7.15) in this case similarly. □

By Corollary 7.4, the following result is a straightforward consequence of Theorem 7.9.

Corollary 7.13. *Let $G_i = (V_i, E_i), i = 1, 2$ be two locally finite simple graphs. Then we have, for any $x \in V_1, y \in V_2$ and $\mathcal{N} \in (0, \infty]$,*

$$\mathcal{K}_{G_1 \times G_2,(x,y)}(\mathcal{N}) \leq \min\{\mathcal{K}_{G_1,x}(\mathcal{N}), \mathcal{K}_{G_2,y}(\mathcal{N})\}. \tag{7.25}$$

When $\mathcal{N} = \infty$, the equality holds, i.e.,

$$\mathcal{K}_{G_1 \times G_2,(x,y)}(\infty) = \min\{\mathcal{K}_{G_1,x}(\infty), \mathcal{K}_{G_2,y}(\infty)\}. \tag{7.26}$$

By Example 7.8, we derive the following result.

Corollary 7.14. *Let $G_i = (V_i, E_i), i = 1, 2$ be two locally finite simple d-regular, ∞-curvature sharp graphs. If either G_1, G_2 are both triangle free, or, $G_1 = G_2$ with $\#_\Delta(x) \equiv const.$ $\forall x$, then $G_1 \times G_2$ is also ∞-curvature sharp.*

Proof. If G_1, G_2 are both triangle free, we have for $x \in V_1$, $y \in V_2$

$$\mathcal{K}_{G_1,x}(\mathcal{N}) = 2 - \frac{2d_x}{\mathcal{N}}, \;\; \mathcal{K}_{G_2,y}(\mathcal{N}) = 2 - \frac{2d_y}{\mathcal{N}}.$$

Theorem 7.9 and Example 7.8 tells

$$\mathcal{K}_{G_1 \times G_2,(x,y)} = 2 - \frac{2(d_x + d_y)}{\mathcal{N}}.$$

That is, (x, y) is ∞-curvature sharp, since $G_1 \times G_2$ is also triangle free. The other case can be shown similarly. $\square$

Corollary 7.14 implies, for example, the Cartesian product of the crown graph Crown(n, n) and the complete bipartite graph $K_{m,m}$ is ∞-curvature sharp. The Cartesian product of $K_n, n \geq 2$ with itself is ∞-curvature sharp. In fact, the latter is the line graph of $K_{n,n}$, which will be discussed in detail in the next subsection.

7.3. **Examples.** In this subsection, we present examples illustrating how Theorem 7.9 can be used to calculate explicit curvature functions.

Example 7.15 (Hypercubes)**.** An n-dimensional hypercube $Q^n = (V, E)$, $n \geq 1, n \in \mathbb{Z}$, is the Cartesian product $\underbrace{K_2 \times \cdots \times K_2}_{n}$. For any $x \in V$, we have

$$\mathcal{K}_{Q^n,x}(\mathcal{N}) = 2 - \frac{2n}{\mathcal{N}} \quad \forall\, \mathcal{N} \in (0, \infty]. \tag{7.27}$$

Proof. Recall from Example 5.17 that the two vertices in K_2 has the same curvature function

$$\mathcal{K}_{K_2,\cdot}(\mathcal{N}) = 2 - \frac{2}{\mathcal{N}} \quad \forall\, \mathcal{N} \in (0, \infty].$$

By Theorem 7.9, and the associativity of $*$-product, we know $\mathcal{K}_{Q^n,x} = \mathcal{K}_{K_2,\cdot} * \cdots * \mathcal{K}_{K_2,\cdot}$. Hence, (7.27) follows from (7.10). $\square$

8. Curvature and spectral gaps at $\mathbf{S_1}$-out regular vertices

Let $G = (V, E)$ be a locally finite simple graph and $x \in V$. We assume henceforth that x is an S_1-out regular vertex of degree $d = d_x \geq 2$, i.e., $d^+_{y_j} = av^+_1(x)$ for all neighbours $y_1, y_2, \ldots, y_d$ of x in G. Recall from Corollary 5.11 that S_1-out regularity of x is equivalent to $\mathcal{N}$-curvature sharpness for some $\mathcal{N} \in (0, \infty]$.

Recall also that we provided an explicit expression for the curvature function at an S_1-out regular vertex x in Theorem 5.7 in terms of the lowest eigenvalue of a matrix $\mathcal{P}_\infty(x)$. Our aim in this section is to express $\mathcal{P}_\infty(x)$ via suitable Laplacians, defined on graphs with vertex set $S_1(x)$. Our main result is Theorem 8.1 below. This theorem implies a quantitative version of Theorem 6.4 in the special case of S_1-out regularity (see Corollary 8.4). We will also use this result to deal with the example of Johnson graphs and will finish this section with specific cardinality estimates of 2-spheres $S_2(x)$ of S_1-out regular vertices $x \in V$.

Let $\Delta_{S_1(x)}$ be the non-normalized Laplacian of the subgraph $S_1(x)$ induced by the vertices $\{y_1, \ldots, y_d\}$, i.e., written as an operator,

$$\Delta_{S_1(x)} f(y_i) = \left(\sum_{j \neq i} w_{y_i y_j} f(y_j) \right) - d^0_{y_i} f(y_i).$$

Let $S'_1(x)$ be the graph with the same vertex set $\{y_1, \ldots, y_d\}$ and an edge between y_i and y_j iff $\#\{z \in S_2(x) \mid y_i \sim z \sim y_j\} \geq 1$, where $\sim$ describes adjacency in the original graph G. We introduce the following weights $w'_{y_i y_j}$ on the edges of $S'_1(x)$:

$$w'_{y_i y_j} = \sum_{z \in S_2(x)} \frac{w_{y_i z} w_{z y_j}}{d^-_z}.$$

The corresponding weighted Laplacian is then given by

$$\Delta_{S_1'(x)} f(y_i) = \left(\sum_{j \neq i} w'_{y_i y_j} f(y_j) \right) - d'_{y_i} f(y_i),$$

where

$$d'_{y_i} = \sum_{z \in S_2(x)} \frac{w_{y_i z}}{d_z^-} \sum_{j \neq i} w_{z y_j} = av_1^+(x) - \sum_{z \in S_2(x), z \sim y_i} \frac{1}{d_z^-}.$$

Let $S_1''(x) = S_1(x) \cup S_1'(x)$, i.e., the vertex set of $S_1''(x)$ is $\{y_1, \dots, y_{d_x}\}$ and the edge set is the union of the edge sets of $S_1(x)$ and $S_1'(x)$. Then the sum $\Delta_{S_1(x)} + \Delta_{S_1'(x)}$ can be understood as the weighted Laplacian $\Delta_{S_1''(x)}$ on $S_1''(x)$ with weights $w'' = w + w'$. Note that all our Laplacians Δ are defined on functions on the vertex set of $S_1(x)$. They are non-positive operators, by definition, and we refer to their eigenvalues λ as solutions of $\Delta f + \lambda f = 0$, to make these eigenvalues non-negative. We denote and order these eigenvalues (with their multiplicities) by

$$0 = \lambda_0(\Delta) \leq \lambda_1(\Delta) \leq \cdots \leq \lambda_{d-1}(\Delta).$$

The second-smallest eigenvalue $\lambda_1(\Delta) \geq 0$ is also called the *spectral gap* of Δ and plays an important role in spectral graph theory. With these operators in place, we have

$$\mathcal{P}_\infty(x) = -4\Delta_{S_1''(x)} - 2(dI_d - J_d),$$

and Theorem 5.7 implies that

$$\mathcal{K}_{G,x}(\mathcal{N}) = \frac{3 + d - av_1^+(x)}{2} - \frac{2d}{\mathcal{N}} + 2 \underbrace{\lambda_{\min} \left(-\Delta_{S_1''(x)} + \left(\frac{1}{\mathcal{N}} - \frac{1}{2} \right) (dI_d - J_d) \right)}_{\leq 0}.$$

Then we have

$$\lambda_{\min} \left(-\Delta_{S_1''(x)} + \left(\frac{1}{\mathcal{N}} - \frac{1}{2} \right) (dI_d - J_d) \right) = \begin{cases} 0, & \text{if } \lambda_1 \geq \frac{d}{2} - \frac{d}{\mathcal{N}}, \\ \lambda_1 + \left(\frac{d}{\mathcal{N}} - \frac{d}{2} \right), & \text{if } \lambda_1 < \frac{d}{2} - \frac{d}{\mathcal{N}}. \end{cases}$$

This leads directly to the following result.

Theorem 8.1. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$ be an S_1-out regular vertex of degree $d \geq 2$. Let $\Delta_{S_1''(x)}$ be the weighted Laplacian defined above with second-smallest eigenvalue $\lambda_1 = \lambda_1(\Delta_{S_1''(x)})$.*

(a) *The case $\lambda_1 \geq \frac{d}{2}$ is equivalent to ∞-curvature sharpness of x. Then we have*

$$\mathcal{K}_{G,x}(\mathcal{N}) = \frac{3 + d - av_1^+(x)}{2} - \frac{2d}{\mathcal{N}}.$$

(b) *If $\lambda_1 < \frac{d}{2}$, we have*

$$\mathcal{K}_{G,x}(\mathcal{N}) = \begin{cases} \frac{3+d-av_1^+(x)}{2} - \frac{2d}{\mathcal{N}}, & \text{if } \mathcal{N} \leq \frac{2d}{d-2\lambda_1}, \\ \frac{3-d-av_1^+(x)}{2} + 2\lambda_1, & \text{if } \mathcal{N} > \frac{2d}{d-2\lambda_1}. \end{cases}$$

Remark 8.2. In certain cases, it is advantageous to use the decomposition $\Delta_{S_1''(x)} = \Delta_{S_1(x)} + \Delta_{S_1'(x)}$ and to investigate the spectral gaps $\lambda_1(\Delta_{S_1(x)})$ and $\lambda_1(\Delta_{S_1'(x)})$ separately, making use of specific geometric properties of the graphs $S_1(x)$ and $S_1'(x)$. The following examples illustrate this point.

Examples 8.3. Let x be a S_1-out regular vertex of the graph $G = (V, E)$ of degree $d \geq 2$.

(a) In our first example we assume $S_1(x) = K_d$ and $S_2(x) = \emptyset$. (This means that $G = K_{d+1}$.) In this case, $S_1'(x)$ is totally disconnected and $\Delta_{S_1''(x)} = \Delta_{S_1(x)}$. The eigenvalues of the non-normalized Laplacian Δ_{K_n} on the complete graph K_d are known to be $\lambda_0(\Delta_{K_n}) = 0$ and $\lambda_1(\Delta_{K_n}) = \cdots = \lambda_{d-1}(\Delta_{K_n}) = d$ and, therefore, Theorem 8.1 yields

$$\mathcal{K}_{G,x}(\mathcal{N}) = \frac{3+d}{2} - \frac{2d}{\mathcal{N}},$$

confirmed by Example 5.17.

(b) Next, we assume $S_1(x)$ to be totally disconnected (i.e., $\#_\Delta(x) = 0$) and $|S_2(x)| = \binom{d}{2}$, where every pair of vertices $y, y' \in S_1(x)$ is connected to precisely one vertex $z \in S_2$ with $d_z^- = 2$. Then $\Delta_{S_1''(x)} = \Delta_{S_1'(x)}$ and $\Delta_{S_1'(x)}$ agrees with $\frac{1}{2}\Delta_{K_n}$. Therefore, we have $\lambda_1(\Delta_{S_1''(x)}) = d/2$ and $av_1^+(x) = d - 1$, and Theorem 8.1 yields

$$\mathcal{K}_{G,x}(\mathcal{N}) = 2 - \frac{2d}{\mathcal{N}}.$$

(c) Finally, we assume $S_1(x)$ to be totally disconnected and $|S_2(x)| = 1$, i.e., $S_2(x) = \{z\}$, where every vertex $y \in S_1(x)$ is connected to z. Then $\Delta_{S_1''(x)} = \Delta_{S_1'(x)}$ and $\Delta_{S_1'(x)}$ agrees with $\frac{1}{d}\Delta_{K_n}$. Therefore, we have $\lambda_1(\Delta_{S_1''(x)}) = 1 \leq d/2$ and $av_1^+(x) = 1$, and Theorem 8.1 yields

$$\mathcal{K}_{G,x}(\mathcal{N}) = \begin{cases} \frac{2+d}{2} - \frac{2d}{\mathcal{N}} & \text{if } \mathcal{N} \leq \frac{2d}{d-2}, \\ \frac{6-d}{2} & \text{if } \mathcal{N} > \frac{2d}{d-2}. \end{cases}$$

An immediate consequence of Theorem 8.1 is a stronger quantitative version of Theorem 6.4 from Section 6 in the case of S^1-out regularity.

Corollary 8.4. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$ an S_1-*out regular *vertex. If $\mathring{B}_2(x)$ has more than one connected component then*

$$\mathcal{K}_{G,x}(\mathcal{N}) = \begin{cases} \frac{3+d-av_1^+(x)}{2} - \frac{2d}{\mathcal{N}}, & \text{if } \mathcal{N} \leq 2, \\ \frac{3-d-av_1^+(x)}{2}, & \text{if } \mathcal{N} > 2. \end{cases}$$

In particular, we have

$$\mathcal{K}_{G,x}(\infty) = \frac{3 - d - av_1^+(x)}{2},$$

and $\mathcal{K}_{G,x}(\infty) < 0$ except for the four cases (a), (c), (d), and (e) presented in Figure 6.

Proof. Note that if $\mathring{B}_2(x)$ has more than one connected component then $d \geq 2$ and $S_1''(x)$ has also more than one connected component. This implies that the eigenvalue 0 of $\Delta_{S_1''(x)}$ has multiplicity at least 2. Then we can apply Theorem 8.1 with $\lambda_1 = 0 < d/2$. The case analysis for $3-d-av_1^+(x) \geq 0$ is very similar as in the proof of Theorem 6.4. $\square$

Another straightforward consequence of Theorem 8.1 is the following.

Corollary 8.5. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$ be an S_1-out regular vertex of degree $d \geq 2$. Let $\lambda_1 \geq 0$ be the second-smallest eigenvalue of $\Delta_{S_1''(x)}$. Then $\mathcal{K}_{G,x}(\infty) \geq 0$ is equivalent to*

$$av_1^+(x) \leq 3 + d \quad \text{and } \lambda_1 \geq \frac{d + av_1^+(x) - 3}{4}. \tag{8.1}$$

In particular, we have $\mathcal{K}_{G,x}(\infty) \geq 0$ if $av_1^+(x) \leq 3 + d$ and $\lambda_1 \geq d/2$. (Note that the second condition is equivalent to ∞-curvature sharpness.)

Remark 8.6. The importance of Corollary 8.5 is that it relates *non-negativity of the curvature* at a vertex $x \in V$ to a large enough *spectral gap* of the weighted Laplacian $\Delta_{S_1''(x)}$ on the 1-sphere $S_1(x)$ in the case of S_1-out regularity.

Using Theorem 8.1, we can show all Johnson graphs are ∞-curvature sharp, which is an extension of Example 5.17.

Example 8.7 (Johnson graphs)**.** Johnson graph $J(n,k)$ is the graph with the set of k-element subsets of an n-element set as the vertex set, where two k-element subsets are adjacent when they have $k-1$ elements in common, see, e.g., [7, Section 12.4.2]. In particular, $J(n,1)$ is the complete graph K_n, and $J(n,2)$ is the line graph $L(K_n)$ of K_n. Each Johnson graph $J(n,k)$ is ∞-curvature sharp. Moreover, for any vertex x of $J(n,k)$, the curvature function is given by

$$\mathcal{K}_{J(n,k),x}(\mathcal{N}) = \frac{n+2}{2} - \frac{2k(n-k)}{\mathcal{N}} \quad \forall\, \mathcal{N} \in (0,\infty]. \tag{8.2}$$

Proof. Denote the n-element set by $[n] := \{1,2,\ldots,n\}$. Let vertex x be the k-element subset $\{i_1, i_2, \ldots, i_k\} \subset [n]$. Then the vertices in $S_1(x)$ can be listed as

$$y_{\ell,m} := \{i_1, \ldots, \widehat{i_\ell}, \ldots, i_k, j_m\}, \quad \ell \in [k],\ m \in [n-k],$$

where $\{j_1, \ldots, j_{n-k}\}$ is the complement of x in $[n]$. By a hat, we mean to delete the corresponding element from the set. Therefore, we have $d := d_x = k(n-k)$.

Any vertex $y_{\ell,m} \in S_1(x)$ is adjacent to the following vertices in $S_2(x)$:

$$z_{\ell,\ell',m,m'} := \{i_1, \ldots, \widehat{i_\ell}, \ldots, \widehat{i_{\ell'}}, \ldots, i_k, j_m, j_{m'}\},\ \ell' \in [k] \setminus \{\ell\},\ m' \in [n-k] \setminus \{m\}.$$

Therefore, $J(n,k)$ is S_1-out regular at x with $av_1^+(x) = (k-1)(n-k-1)$. This implies

$$\mathcal{K}_\infty^0(x) := \frac{3 + d_x - av_1^+(x)}{2} = \frac{n+2}{2}.$$

Any vertex $z_{\ell,\ell',m,m'} \in S_2(x)$ is adjacent to $y_{\ell,m}$, $y_{\ell',m}$, $y_{\ell,m'}$, $y_{\ell',m'} \in S_1(x)$. That is, vertices in $S_2(x)$ have constant in degree 4.

We now figure out the weighted Laplacian $\Delta_{S_1''(x)}$. First observe that two vertices $y_{\ell_1,m_1}, y_{\ell_2,m_2} \in S_1(x)$ are adjacent if and only if

$$\ell_1 = \ell_2,\ m_1 \neq m_2 \quad \text{or} \quad \ell_1 \neq \ell_2,\ m_1 = m_2.$$

That is, the subgraph $S_1(x)$ is the Cartesian product $K_k \times K_{n-k}$ of two complete graphs. When $\ell_1 = \ell_2 := \ell$, $m_1 \neq m_2$, $y_{\ell_1,m_1}, y_{\ell_2,m_2}$ have $k-1$ common neighbours in $S_2(x)$: z_{ℓ,ℓ',m_1,m_2}, $\ell' \in [k] \setminus \{\ell\}$. When $\ell_1 \neq \ell_2$, $m_1 = m_2 := m$, $y_{\ell_1,m_1}, y_{\ell_2,m_2}$ have $n-k-1$ common neighbours in $S_2(x)$: $z_{\ell_1,\ell_2,m,m'}$, $m' \in [n-k] \setminus \{m\}$.

Furthermore, any two vertices $y_{\ell_1,m_1}, y_{\ell_2,m_2} \in S_1(x)$ with $\ell_1 \neq \ell_2$, $m_1 \neq m_2$ has exactly one common neighbour in $S_2(x)$, that is, $z_{\ell_1,\ell_2,m_1,m_2}$. We like to mention that pairs of vertices of this kind are not adjacent in the subgraph $S_1(x)$.

We denote the weighted complete graph K_k with constant edge weight c_1 by (K_k, c_1). Let $(K_k, c_1) \times (K_{n-k}, c_2)$ be the weighted Cartesian product $K_k \times K_{n-k}$, whose edge weights are naturally inherited from (K_k, c_1) and (K_{n-k}, c_2). Then we have

$$\begin{aligned}\Delta_{S_1''(x)} &= \Delta_{(K_d, \frac{1}{4})} + \Delta_{(K_k, 1+\frac{n-k-1}{4}-\frac{1}{4}) \times (K_{n-k}, 1+\frac{k-1}{4}-\frac{1}{4})} \\ &= -\frac{1}{4}(dI_d - J_d) + \Delta_{(K_k, \frac{n-k+2}{4}) \times (K_{n-k}, \frac{k+2}{4})}.\end{aligned}$$

Recalling that the Laplacian eigenvalues of the Cartesian product are given by all possible sums of the Laplacian eigenvalues of the two original graphs, it is straightforward to check

$$\lambda_1(\Delta_{S_1''(x)}) = \min\left\{\frac{k(n-k+1)}{2}, \frac{(n-k)(k+1)}{2}\right\} > \frac{k(n-k)}{2} = \frac{d}{2}.$$

Therefore, we conclude from Theorem 8.1 that $J(n,k)$ is ∞-curvature sharp, and the curvature function (8.2) then follows immediately. $\square$

Remark 8.8. From (8.2), we see the graphs $J(n,k)$ and $J(n,n-k)$ share the same curvature function. In fact, they are isomorphic. The isomorphism is given by sending a k-element subset to its complement. Johnson graphs have many other interesting properties. They are distance-regular, but not always strongly regular. The diameter of $J(n,k)$ is $\min\{k, n-k\}$. Johnson graphs are important in translating many combinatorial problems about sets into graph theory. We refer to [7, Section 12.4.2], [15, Section 1.6] for more discussions.

We finish this section by a discussion of upper bounds for the cardinality of $S_2(x)$. A trivial upper bound, assuming nothing besides the S_1-regularity of x, is given by

$$|S_2(x)| \leq d \cdot av_1^+(x). \tag{8.3}$$

This estimate does not take into account that different vertices of $S_1(x)$ may be connected to the same vertex in $S_2(x)$. The next result gives another upper bound in terms of the spectral gap. This result is sometimes better than (8.3) and, at other times, worse.

Proposition 8.9. *Let $G = (V,E)$ be a locally finite simple graph and $x \in V$ be an S_1-out regular vertex of degree $d \geq 2$. Let $\lambda_1 \geq 0$ be the second-smallest eigenvalue of $\Delta_{S_1''(x)}$. Then we have*

$$|S_2(x)| \leq \left(\sum_{j=1}^{d}(d_{y_j} - 1)\right) - (d-1)\lambda_1.$$

Note that $\sum_{j=1}^{d}(d_{y_j} - 1)$ would be the cardinality of $|S_2(x)|$ in the case when $B_2(x)$ were a tree.

Proof. Let $\lambda_0 = 0 \leq \lambda_1 \leq \cdots \leq \lambda_{d-1}$ be the eigenvalues of $\Delta_{S_1''(x)}$. Then we have

$$(d-1)\lambda_1 \leq \sum_{j=1}^{d-1}\lambda_j = \mathrm{Trace}(-\Delta_{S_1''(x)}) = \left(\sum_{j=1}^{d} d_{y_j}^0\right) + \left(\sum_{j=1}^{d} d'_{y_j}\right).$$

For the second sum on the right hand side we obtain

$$\sum_{j=1}^d d'_{y_j} = \sum_{j=1}^d \left(av_1^+(x) - \sum_{z\in_2(x), z\sim y_j} \frac{1}{d_z^-} \right) =$$

$$= dav_1^+(x) - \sum_{z\in S_2(x)} \sum_{j:y_j\sim z} \frac{1}{d_z^-} = dav_1^+(x) - |S_2(x)|.$$

Combination with the first sum on the right hand side leads to

$$(d-1)\lambda_1 \leq \left(\sum_{j=1}^d (d_{y_j} - 1) \right) - |S_2(x)|. \tag{8.4}$$

Rearranging this inequality finishes the proof. □

Combining Proposition 8.9 with inequality (8.1) leads directly to the following result in the case of non-negative curvature.

Corollary 8.10. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$ be an S_1-out regular vertex of degree $d \geq 2$ satisfying $\mathcal{K}_{G,x}(\infty) \geq 0$. Then we have $av_1^+(x) \leq d + 3$ and*

$$|S_2(x)| \leq \left(\sum_{j=1}^d (d_{y_j} - 1) \right) - (d-1)\frac{d + av_1^+(x) - 3}{4}.$$

This simplifies in the case of a d-regular graph to

$$|S_2(x)| \leq (d-1)\left(\frac{3}{4}d - \frac{av_1^+(x) - 3}{4} \right).$$

Note in comparison that the 2-sphere of a d-regular tree has cardinality $(d-1)d$. Another immediate consequence is the following result.

Corollary 8.11. *Let $G = (V, E)$ be a locally finite simple graph and $x \in V$ be an S_1-out regular vertex of degree $d \geq 2$. If x is* ∞-curvature sharp*, we have*

$$|S_2(x)| \leq \left(\sum_{j=1}^d (d_{y_j} - 1) \right) - \frac{d(d-1)}{2}.$$

This, together with our trivial estimate (8.3) *yields, in the case of a d-regular graph*

$$|S_2(x)| \leq \min\left\{ \frac{d(d-1)}{2}, d \cdot av_1^+(x) \right\}.$$

Proof. Recall that ∞-curvature sharpness of x is equivalent to $\lambda_1 \geq d/2$. Then apply Proposition 8.9. □

Remark 8.12. (a) The ∞-curvature sharpness condition at a vertex x implies for d-regular graphs that the cardinality of $|S_2(x)|$ is at most half as large as the corresponding 2-sphere of a d-regular tree. Tightness of this estimate was obtained in Example 8.3(b).

(b) Note that in the case of a d-regular graph $G = (V, E)$ the inequalities (8.1) and (8.4) can also be understood as the following bounds of the spectral gap of $\Delta_{S_1''(x)}$ at an S_1-out regular vertex $x \in V$ with $\mathcal{K}_{G,x}(\infty) \geq 0$:

$$\frac{d}{4} + \frac{av_1^+(x) - 3}{4} \leq \lambda_1 \leq d - \frac{1}{d-1}|S_2(x)|.$$

Moreover, the upper bound for λ_1 holds generally without any curvature restriction.

9. Curvature of Cayley graphs

It is a well known general fact that all abelian Cayley graphs or, more generally, all Ricci-flat graphs lie in the class $CD(0, \infty)$ [11, 25]. In this section, we will consider more subtle curvature properties of abelian and especially also non-abelian Cayley graphs.

Generally, a Cayley graph $G = \mathrm{Cay}(\Gamma, S)$ is determined by a discrete group Γ and a finite set of generators $S \subset \Gamma$ which is symmetric (i.e., if $s \in S$ then also $s^{-1} \in S$). The vertices of a Cayley graph are the elements of Γ and every directed edge can be labelled by one of the generators in S.

Henceforth, $e \in \Gamma$ denotes the identity element and S does never contain e (which would give rise to a loop). Note that if a generator $s \in S$ has order 2, i.e., if $s = s^{-1}$, this element is contained only once in S and gives rise to a single edge emanating from any given vertex, and labelled in both directions by s. Any non-empty word $r(S)$ in the generators S is called a *relation* if it represents the identity element. Geometrically, every relation corresponds one-to-one to a closed walk in the corresponding Cayley graph starting from and returning to, say, the identity $e \in \Gamma$. We call a relation *reduced*, if it does not contain a subword of the form ss^{-1}. Geometrically, the corresponding closed walk is without backtracking. Note that Cayley graphs are $|S|$-regular and vertex transitive. Since every regular graph without triangles is S^1-out regular, the same holds true for Cayley graphs $\mathrm{Cay}(\Gamma, S)$ which do not have relations of length 3. Most of our examples of Cayley graphs will have this property.

Since all vertices have the same curvature function, we can drop the reference to the vertex and simply write $\mathcal{K}_G$ for $\mathcal{K}_{G,e}$.

We start by presenting a general family of abelian Cayley graphs having precisely zero curvature at infinity.

Theorem 9.1. *Let $G = \mathrm{Cay}(\Gamma, S)$ be an abelian Cayley graph with $2m = |S| \geq 2$. If all reduced relations of S have length ≥ 5 except for the relations $s_1 s_2 s_1^{-1} s_2^{-1}$ expressing the commutativity, then we have for all $g \in \Gamma$*

$$\mathcal{K}_G(\mathcal{N}) = \begin{cases} 2 - \frac{4m}{\mathcal{N}}, & \text{if } \mathcal{N} \leq 2m, \\ 0, & \text{if } \mathcal{N} > 2m. \end{cases}$$

In particular, we have $\mathcal{K}_G(\infty) = 0$.

Proof. First recall that G is d-regular with $d = 2m$.

If S contains an element $s \in S$ of order $k \leq 4$, the word s^k is a reduced relation of length ≤ 4. Therefore, all elements of S have oder at least 5.

Next we describe the structure of $\mathring{B}_2(e)$: We have $S_1(e) = S$ with no edges between two different vertices of $S_1(e)$. A pair of vertices $s_1, s_2 \in S_1(e)$ is connected via a unique vertex $s_1 s_2 = s_2 s_1$ in $S_2(e)$ iff $s_1 \neq s_2^{-1}$. Otherwise s_1 and s_2 are not connected via a vertex in $S_2(e)$. Moreover, every vertex $s \in S_1(e)$ is adjacent to its square $s^2 \in S_2(x)$. Since G is S_1-out regular (it does not have relations of length 3), we can apply the results of section 8. In particular, we have $av_1^+(e) = 2m - 1$ and $d^-_{s_1 s_2} = 2$ and $d^-_{s^2} = 1$ for $s_1, s_2, s \in S$ with $s_1 \neq s_2^{\pm 1}$. As a consequence, $S_1'(e) = S_1''(e)$ is the *cocktail party graph* of $2m = |S|$ vertices. The spectrum of the adjacency matrix $A_{S_1''(e)}$ of $S_1''(e)$ is known to be (see [7, Section 8.1])

$$\sigma(A_{S_1''(e)}) = \{\underbrace{-2, \dots, -2}_{m-1}, \underbrace{0, \dots, 0}_{m}, 2m-2\}.$$

The weights of the weighted Laplacian $\Delta_{S_1''(e)}$ are all equal to $1/2$ and, therefore, we have $\lambda_1(\Delta_{S_1''(e)}) = m - 1 < d/2 = m$. Note that $3 + d - av_1^+(x) = 4$ and Theorem 8.1(b) tells us that

$$\mathcal{K}_G(\mathcal{N}) = \begin{cases} 2 - \frac{4m}{\mathcal{N}}, & \text{if } \mathcal{N} \le 2m, \\ 0, & \text{if } \mathcal{N} > 2m. \end{cases}$$

□

Remark 9.2. In fact, there exists an absolute constant C such that for any abelian Cayley graph $G = Cay(\Gamma, S)$ with degree $d = |S|$ and size N, we have

$$0 \le \mathcal{K}_G(\infty) \le CdN^{-\frac{4}{d}}. \tag{9.1}$$

In particular, when the size $N \to \infty$, $\mathcal{K}_G(\infty)$ tends to zero. This follows from two estimates for the eigenvalue $\lambda_1(\Delta)$ of the Laplacian Δ of G: A Lichnerowicz type estimate (see [10, 21]) tells $\lambda_1(\Delta) \ge \mathcal{K}_G(\infty)$; Friedman, Murty, and Tillich [14] prove that there exists an absolute constant C such that for any abelian Cayley graph, $\lambda_1(\Delta) \le CdN^{-\frac{4}{d}}$.

Now we move on to general Cayley graphs which are no longer assumed to be abelian. All our groups Γ are finitely presented, i.e., $\Gamma = \langle S \mid R \rangle$, where $S \subset \Gamma \setminus \{e\}$ is finite and symmetric and R consists of finitely many words $r_1(S), \dots, r_N(S)$, the so-called *defining relations* of (the presentation of) Γ. We conjecture that the curvature function behaves monotonically under addition of defining relations:

Conjecture 9.3. Let Γ be given by

$$\Gamma = \langle S \mid r_1(S), \dots, r_N(S) \rangle,$$

and Γ' be another group, differing from Γ by one additional defining relation:

$$\Gamma' = \langle S \mid r_1(S), \dots, r_N(S), r'(S) \rangle.$$

Assume that none of the generators in $S \subset \Gamma$ is redundant in Γ', i.e., for any two different generators $s_1, s_2 \in S$ in the original group Γ we also have $s_1 \ne s_2$ in Γ' and $s_1 \ne e_{\Gamma'} \ne s_2$.

Then the associated Cayley graphs $G = \mathrm{Cay}(\Gamma, S)$ and $G' = \mathrm{Cay}(\Gamma', S)$ are both $|S|$-regular and we have:

$$\mathcal{K}_{G'}(\mathcal{N}) \ge \mathcal{K}_G(\mathcal{N}) \quad \text{for all } \mathcal{N} \in (0, \infty].$$

Example 9.4. The Cayley graph G of the free abelian group $\Gamma = \langle \{a^{\pm 1}\} \mid \emptyset \rangle$ is the 2-regular tree T_2. Theorem 9.1 tells us that

$$\mathcal{K}_G(\mathcal{N}) = \mathcal{K}_{T_2}(\mathcal{N}) = \begin{cases} 2 - \frac{4}{\mathcal{N}}, & \text{if } \mathcal{N} \le 2, \\ 0, & \text{if } \mathcal{N} > 2. \end{cases}$$

Let

$$\Gamma' = \langle \{a^{\pm 1}\} \mid a^k \rangle \tag{9.2}$$

for some $k \geq 3$. The corresponding Cayley graph agrees with the k-cycle C_k, and Example 5.20 shows that

$$\mathcal{K}_{C_3}(\mathcal{N}) \geq \mathcal{K}_{C_4}(\mathcal{N}) \geq \mathcal{K}_{C_n}(\mathcal{N}) = \mathcal{K}_{T_2}(\mathcal{N})$$

for all $n \geq 5$. If we choose $k = 1$ or $k = 2$ in (9.2), the original generator set $S = \{a^{\pm 1}\}$ becomes redundant in Γ' since then $a = e$ or $a = a^{-1}$, respectively.

Here is another fact supporting the above conjecture.

Proposition 9.5. *Let Γ and Γ' be defined as in Conjecture 9.3. If every reduced relation $r(S)$ of Γ' which is not a relation of Γ (i.e., does not represent the identity in Γ) has length at least ≥ 4, then the statement of the conjecture is true. (We refer to these relations as* new relations *in Γ'. Note this property is required for* all *relations of Γ' and not only for the defining ones.)*

Proof. The additional defining relation $r'(S)$ of Γ' leads to a surjective group homomorphism $\Gamma \to \Gamma'$. Correspondingly, there is a map from the vertices of the Cayley graph G to the vertices of the Cayley graph G'. The non-redundancy condition on the set S of generators implies that this map is a bijection between the 1-balls $B_1^G(e)$ and $B_1^{G'}(e)$. Generally, different elements in Γ may be mapped to the same element in Γ'. On the Cayley graph level, this corresponds to a merging/identification of different vertices in G to end up with the graph G'. For our curvature consideration, we are only concerned with identifications appearing inside the punctured 2-balls of the identities. The condition on the length of new relations guarantees that such an identification affects only vertices in the 2-spheres $S_2^G(e)$ and $S_2^{G'}(e)$ (since any identification of a vertex in $B_2^G(e)$ with a vertex in $B_1^G(e)$ would correspond to a new relation of length ≤ 3 in Γ'). Therefore, the transition from $\mathring{B}_2^G(x)$ to $\mathring{B}_2^{G'}(x)$ can be described via a succession of mergings of pairs of vertices in the 2-sphere. Since the directed edges of both Cayley graphs G and G' are labelled by elements of S, two different vertices can only be merged if they do not have common neighbours. This allows us to apply Proposition 6.12 repeatedly and we conclude that we have

$$\mathcal{K}_{G'}(\mathcal{N}) \geq \mathcal{K}_G(\mathcal{N})$$

for any $\mathcal{N} \in (0, \infty]$. □

Dihedral groups D_{2k} are examples of *Coxeter groups*. Coxeter groups are groups W with generators $S = \{s_1, \dots, s_k\}$ and presentations

$$W = \langle S \mid (s_i s_j)^{m(i,j)} \rangle, \tag{9.3}$$

where $m(i,i) = 1$ and $m(i,j) \geq 2$ for all $i \neq j$. It is also possible to choose $m(i,j) = \infty$, which means that there is no relation between the generators s_i and s_j. The condition $m(i,i) = 1$ means that each generator s_i has order 2, and the condition $m(i,j) = 2$ means that the generators s_i and s_j commute. To a given Coxeter group (9.3), we associate a Coxeter diagram (also called Dynkin diagram) as follows: It is a finite graph with k vertices (every vertex represents a generator s_j) and the vertices corresponding to s_i and s_j are connected by an edge if and only if $m(i,j) \geq 3$. For example, the Coxeter diagram of the dihedral group

$$D_{2k} = \langle \{s_1, s_2\} \mid s_1^2, s_2^2, (s_1 s_2)^k \rangle$$

is the complete graph K_2. The Coxeter diagram carries all information to calculate the curvature function of the Cayley graph $\mathrm{Cay}(W, S)$.

Theorem 9.6. *Let (W,S) be a Coxeter group as defined in (9.3) with $k = |S|$. Assume that the corresponding Coxeter diagram has at least one edge. Let $\mu^{max}(W,S) \in (0,k]$ be the maximal eigenvalue of the non-normalized Laplacian on the corresponding Coxeter diagram. Then the curvature function of $G = \mathrm{Cay}(W,S)$ is given by*

$$\mathcal{K}_G(\mathcal{N}) = \begin{cases} 2 - \frac{2k}{\mathcal{N}}, & \text{if } \mathcal{N} \le \mathcal{N}_0, \\ 2 - \mu^{max}(W,S), & \text{if } \mathcal{N} > \mathcal{N}_0, \end{cases}$$

with $\mathcal{N}_0 = 2k/\mu^{max}(W,S)$.

Proof. Let (W,S) be a Coxeter group as defined in (9.3) and $G = \mathrm{Cay}(W,S)$ be the associated Cayley graph.

We extend first the notion of a *reduced relation* to be any relation which does neither contain subwords of the form ss^{-1} nor of the form s^2 for $s \in S$ (since $s^{-1} = s$). Then the Coxeter group (W,S) does not have any non-trivial reduced relation of length ≤ 4 other than $(s_is_j)^{m(i,j)}$ with $m(i,j) = 2$. This is a direct consequence of Tits' solution of the word problem for Coxeter groups (see [12, Theorem 3.4.2]). In particular, G is triangle free and S^1-out regular with $av_1^+(e) = k-1$. The induced subgraph $S_1(e)$ of G does not have any edges and its vertices correspond to the generators in S. Moreover, two different vertices $s_i, s_j \in S$ are connected by an edge in $S_1'(e) = S_1''(e)$ if and only if $m(i,j) = 2$ (since the relation $(s_is_j)^2$ means in the original graph G that s_i and s_j have the unique common neighbour $s_is_j = s_js_i$ in $S_2(e)$). This implies that $S_1''(e)$ is the complement of the Coxeter diagram. Since the in degree of $s_is_j \in S_2(e)$ in the case $m(i,j) = 2$ is equal to 2, all weights of the weighted Laplacian $\Delta_{S_1''(e)}$ are equal to $1/2$, and we have (see [7, Section 1.3.2] for the spectrum of the complement)

$$\lambda_1 = \lambda_1(\Delta_{S_1''(e)}) = \frac{1}{2}(k - \mu^{max}(W,S)).$$

Since $d = k$, we have $\lambda_1 < d/2$ and the statement of the theorem follows directly from Theorem 8.1(b). □

Remark 9.7. If the Coxeter diagram of (W,S) has no edges, we are in the case of the Coxeter group $A_1^k = A_1 \times \cdots \times A_1$ (with $k = |S|$) and we have $\mu^{max}(W,S) = 0$. It can be checked similarly as above that the Cayley graph $G = \mathrm{Cay}(W,S)$ is then ∞-curvature sharp and

$$\mathcal{K}_G(\mathcal{N}) = 2 - \frac{2k}{\mathcal{N}}.$$

Example 9.8. The Coxeter diagrams of the finite Coxeter group A_n and the affine Coxeter group $\widetilde{A_n}$, $n \ge 2$, are the path P_n and the cycle C_{n+1}.

Let us now calculate the curvature functions of the corresponding Cayley graphs $G_n = \mathrm{Cay}(A_n, \{s_1, \dots, s_n\})$ and $G_n' = \mathrm{Cay}(\widetilde{A_n}, \{s_1, \dots, s_{n+1}\})$. (In the particular case $n = 2$, G_2 is the hexagon C_6 and G_2' can be viewed as the 1-skeleton of the regular hexagonal tiling of $\mathbb{R}^2$.)

The spectrum of the non-normalized Laplacian on P_n is given by $\mu_j = 2 - 2\cos(\pi j/n)$ for $j = 0, 1, \dots, n-1$ (see [7, Section 1.4.4]), and therefore

$$\mu^{max} = 2 - 2\cos(\frac{n-1}{n}\pi).$$

Therefore, we have

$$\mathcal{K}_{G_n}(\mathcal{N}) = \begin{cases} 2 - \frac{2n}{\mathcal{N}}, & \text{if } \mathcal{N} \le \mathcal{N}_0, \\ 2\cos(\frac{n-1}{n}\pi), & \text{if } \mathcal{N} > \mathcal{N}_0, \end{cases}$$

with $\mathcal{N}_0 = n/(1-\cos(\pi(n-1)/n))$. In particular, we have

$$\lim_{n\to\infty} \mathcal{K}_{G_n}(\infty) = -2.$$

The spectrum of the non-normalized Laplacian on C_{n+1} is $\mu_j = 2 - 2\cos(2\pi j/(n+1))$ for $j = 0, 1, \ldots, n$ (see [7, Section 1.4.3]), which implies

$$\mu^{max} = 2 - 2\cos\left(\frac{n+\delta_{odd}(n)}{n+1}\pi\right),$$

with $\delta_{odd}(n) \in \{0,1\}$ taking the value 1 iff n is odd. Therefore, we have

$$\mathcal{K}_{G'_n}(\mathcal{N}) = \begin{cases} 2 - \frac{2(n+1)}{\mathcal{N}}, & \text{if } \mathcal{N} \le \mathcal{N}_0, \\ 2 - 2\cos(\frac{n+\delta_{odd}(n)}{n+1}\pi), & \text{if } \mathcal{N} > \mathcal{N}_0, \end{cases}$$

with $\mathcal{N}_0 = (n+1)/(1-\cos(\pi(n+\delta_{odd}(n))/(n+1)))$. Again we have

$$\lim_{n\to\infty} \mathcal{K}_{G'_n}(\infty) = -2.$$

9.1. **Global structure of graphs satisfying $CD(0,\infty)$.** We end this section by discussing global results and conjectures and present an infinite family of $6-$regular graphs satisfying $CD(0,\infty)$ which are not Cayley graphs.

Embarrassingly, we know very little about the global structure of graphs satisfying $CD(K,\infty)$ for a fixed $K \ge 0$. Let us start with the following two fundamental facts:

(a) The class $CD(K,\infty)$ is closed under taking Cartesian products.
(b) All abelian Cayley graphs lie in the class $CD(0,\infty)$ ([11, 25, 21]).

Some local properties of graphs in the class $CD(0,\mathcal{N})$ for finite dimension $\mathcal{N}$ were already discussed in Section 2.5. One might hope that every graph in $CD(0,\infty)$ lies also in $CD(0,\mathcal{N})$ for some large enough finite $\mathcal{N}$, but we saw that the complete bipartite graph $K_{2,6}$ is a counterexample (see example 2.13). Other local obstructions to satisfy $CD(0,\infty)$ were discussed in Section 6.

It is natural to investigate whether known global results for Riemannian manifolds with lower bounds on their Ricci curvature have analogues in the graph theoretical setting. The following result on the global structure of positively curved graphs can be found in [27] and can be viewed as some analogue of a Bonnet-Myers' Theorem. (It was included as a conjecture in an earlier version of this paper before it became a theorem; back then it was Conjecture 8.1.)

Theorem 9.9 (Corollary 2.2, [27])**.** *Let $G = (V,E)$ be a graph satisfying $CD(K,\infty)$ for $K > 0$. If G has bounded vertex degree $\le d_{\max}$, then G is a finite graph and we have*

$$\text{diam(G)} \le \frac{2d_{\max}}{K}.$$

Examples of finite regular graphs in $CD(2,\infty)$ with increasing diameters are the hypercubes Q_n which are Cartesian products of n copies of K_2. Both the vertex degree and diameter of Q_n is n, showing that the diameter bound in the above theorem must depend on $d_{\max}$.

The following conjecture can be viewed as some analogue of Bishop's Comparison Theorem:

Conjecture 9.10. Let $d_{max} \in \mathbb{N}$. Then every graph $G = (V,E)$ with $d_x \le d_{\max}$ for all $x \in V$ satisfying $CD(0,\infty)$ has polynomial volume growth. Moreover, there are constants $C_1, C_2 > 0$, only depending on d_{max} that for all $x \in V$ and $r \in \mathbb{N}$.

$$|B_r(x)| \le C_1(1 + r^{C_2}).$$

Examples of infinite regular graphs in $CD(0,\infty)$ with polynomial volume growth are abelian Cayley graphs. The dependence on the maximal degree d_{max} follows easily from the construction of taking Cartesian products.

The following conjecture would be a direct consequence of Conjecture 9.10, since the Cheeger isoperimetric constants $h(G_n)$ of increasing d-regular graphs G_n with uniform upper polynomial volume growth must tend to zero.

Conjecture 9.11. Let $d \in \mathbb{N}$. No infinite family of finite increasing d-regular graphs satisfying $CD(0,\infty)$ can be a family of expander graphs.

A corresponding statement for d-regular abelian Cayley graphs is well known ([1]). Therefore, it is natural to ask whether $CD(0,\infty)$ is really a substantially larger class than the class of all abelian Cayley graphs. To finish this section, we present an infinite family of finite increasing 6-regular non-Cayley graphs G_n satisfying $CD(0,\infty)$.

Example 9.12. [Infinite family of 6-regular non-Cayley graphs satisfying $CD(0,\infty)$] Let $G = (V,E)$ be the 4-regular graph introduced in Example 5.12. The curvature calculations there showed that G satisfies $CD(5/2,\infty)$. Let G_n be the Cartesian product of G with the cycle C_n. Since C_n satisfies $CD(0,\infty)$, the graphs G_n are a family of increasing 6-regular graphs satisfying also $CD(0,\infty)$. Each of the graphs G_n is not a Cayley graph.

Proof. From Example 5.20, we see $0 \leq \mathcal{K}_{C_n,\cdot}(\infty)$. Recall from Example 5.12, there are vertices in G with different curvature functions, i.e.,

$$\mathcal{K}_{G,x_1}(\mathcal{N}) = \frac{5}{2} - \frac{8}{\mathcal{N}} \text{ and } \mathcal{K}_{G,y_1}(\mathcal{N}) = 5 - \frac{8+\sqrt{21\mathcal{N}^2+72\mathcal{N}+64}}{2\mathcal{N}}.$$

Note that $\mathcal{K}_{G,x_1}(1) < \mathcal{K}_{G,y_1}(1) < 0 \leq \mathcal{K}_{C_n,\cdot}(\infty)$. We have, by Proposition 7.7,

$$\mathcal{K}_{G,x_1} * \mathcal{K}_{C_n,\cdot} \neq \mathcal{K}_{G,y_1} * \mathcal{K}_{C_n,\cdot}.$$

Therefore, there are vertices in $G_n = G \times C_n$ with different curvature functions. This rules out that any of the graphs G_n is a Cayley graph. □

10. Curvature functions of graphs with general measures

Many of the computing methods for the Bakry-Émery curvature functions discussed above are extendible to the following general setting. Let $G = (V,E)$ be a locally finite simple graph. We can assign a symmetric nonnegative edge weights $w : E \to [0,\infty)$ and a positive vertex measure $\mu : V \to (0,\infty)$. For $\{x,y\} \in E$, we write $w_{xy} = w_{yx}$. (Recall we used a zero/one valued edge weights in (2.8).) We consider the curvature functions corresponding to the following Laplacian:

$$\Delta_{\mu,w} f(x) := \frac{1}{\mu(x)} \sum_{y,y\sim x} w_{xy}(f(y)-f(x)). \tag{10.1}$$

Denote $d_x := \sum_{y,y\sim x} w_{xy}$, and let $S_1(x) = \{y_1,\ldots,y_k\}$. By definition it is straightforward to find the following matrices. We have

$$\Delta_{\mu,w}(x) = \frac{1}{\mu(x)} \begin{pmatrix} -d_x & w_{xy_1} & \cdots & w_{xy_k} \end{pmatrix},$$

and

$$2\Gamma_{\mu,w}(x) = \frac{1}{\mu(x)} \begin{pmatrix} d_x & -w_{xy_1} & \cdots & -w_{xy_k} \\ -w_{xy_1} & w_{xy_1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -w_{xy_k} & 0 & \cdots & w_{xy_k} \end{pmatrix}.$$

The matrix $4\Gamma_2^{full}(x)$ is given entry-wise as follows:

$$(4\Gamma_2^{full}(x))_{x,x} = \frac{d_x^2}{\mu(x)^2} + \frac{3}{\mu(x)} \sum_{y\in S_1(x)} \frac{w_{xy}^2}{\mu(y)},$$

for any $y \in S_1(x)$,

$$\begin{aligned}(4\Gamma_2^{full}(x))_{x,y} =& -\frac{3w_{xy}^2}{\mu(x)\mu(y)} + \frac{w_{xy}}{\mu(x)\mu(y)} \left(\sum_{z\in S_2(x), z\sim y} w_{yz} \right) + \frac{d_x w_{xy}}{\mu(x)^2} \\ & - \frac{1}{\mu(x)} \sum_{y'\in S_1(x), y'\sim y} \left(\frac{w_{xy}w_{yy'}}{\mu(y)} - \frac{w_{xy'}w_{yy'}}{\mu(y')} \right),\end{aligned}$$

$$\begin{aligned}(4\Gamma_2^{full}(x))_{y,y} =& \frac{3w_{xy}^2}{\mu(x)\mu(y)} + \frac{2w_{xy}^2}{\mu(x)^2} - \frac{d_x w_{xy}}{\mu(x)} + \frac{3w_{xy}}{\mu(x)\mu(y)} \sum_{z\in S_2(x), z\sim y} w_{yz} \\ & + \sum_{y'\in S_1(x), y'\sim y} \left(\frac{w_{xy'}w_{yy'}}{\mu(y')} + 3\frac{w_{xy}w_{yy'}}{\mu(y)} \right),\end{aligned}$$

for any $y_i, y_j \in S_1(x)$, $y_i \neq y_j$,

$$(4\Gamma_2^{full}(x))_{y_i,y_j} = 2\frac{w_{xy_i}w_{xy_j}}{\mu(x)^2} - \frac{1}{\mu(x)} \left(\frac{2w_{xy_i}w_{y_iy_j}}{\mu(y_i)} + \frac{2w_{xy_j}w_{y_iy_j}}{\mu(y_j)} \right),$$

and, for any $z \in S_2(x)$,

$$(4\Gamma_2^{full}(x))_{x,z} = (4\Gamma_2^{full}(x))_{z,z} = \frac{1}{\mu(x)} \sum_{y\in S_1(x), y\sim z} \frac{w_{xy}w_{yz}}{\mu(y)},\ (4\Gamma_2^{full}(x))_{y,z} = -\frac{2w_{xy}w_{yz}}{\mu(x)\mu(y)},$$

for any $z_1, z_2 \in S_2(x)$, $z_1 \neq z_2$, $(4\Gamma_2^{full}(x))_{z_1,z_2} = 0$.

When $w \equiv 1$ and $\mu \equiv 1$, it reduces to the non-normalized Laplacian (1.1).

Now we discuss briefly the curvature functions $\mathcal{K}_{G,x}^{nor}(\cdot)$ corresponding to the normalized Laplacian, i.e., the case $w \equiv 1$ and $\mu(x) = d_x\ \forall x \in V$. This provides another interesting special case. Finally, we discuss some further analogous fundamental curvature results in the normalized case.

We have

$$\Delta^{nor}(x) = \frac{1}{d_x} \begin{pmatrix} -d_x & 1 & \cdots & 1 \end{pmatrix},$$

and

$$2\Gamma^{nor}(x) = \frac{1}{d_x} \begin{pmatrix} d_x & -1 & \cdots & -1 \\ -1 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & \cdots & 1 \end{pmatrix}.$$

By using the full formula above the matrix $4\Gamma_2^{nor}(x)$ is given entry-wise as follows:

$$(4\Gamma_2^{nor}(x))_{x,x} = 1 + \frac{3}{d_x}\sum_{y\in S_1(x)}\frac{1}{d_y},$$

for any $y \in S_1(x)$,

$$(4\Gamma_2^{nor}(x))_{x,y} = -\frac{3+d_y+d_y^+}{d_xd_y} - \frac{1}{d_x}\sum_{y'\in S_1(x),y'\sim y}\left(\frac{1}{d_y}-\frac{1}{d_{y'}}\right),$$

$$(4\Gamma_2^{nor}(x))_{y,y} = \frac{2}{d_x^2} + \frac{3-d_y+3d_y^+}{d_xd_y} + \frac{1}{d_x}\sum_{y'\in S_1(x),y'\sim y}\left(\frac{1}{d_{y'}}+\frac{3}{d_y}\right),$$

for any $y_i, y_j \in S_1(x)$, $y_i \neq y_j$,

$$(4\Gamma_2^{nor}(x))_{y_i,y_j} = \frac{2}{d_x^2} - \frac{w_{y_iy_j}}{d_x}\left(\frac{2}{d_{y_1}}+\frac{2}{d_{y_2}}\right),$$

and, for any $z \in S_2(x)$,

$$(4\Gamma_2^{nor}(x))_{x,z} = (4\Gamma_2^{nor}(x))_{z,z} = \frac{1}{d_x}\sum_{y\in S_1(x),y\sim z}\frac{1}{d_y},\ (4\Gamma_2^{nor}(x))_{y,z} = -\frac{2w_{yz}}{d_xd_y},$$

for any $z_1, z_2 \in S_2(x)$, $z_1 \neq z_2$, $(4\Gamma_2^{nor}(x))_{z_1,z_2} = 0$.

We have the following upper bounds.

Theorem 10.1. *Let $G = (V, E)$ be a locally finite simple graph and let $x \in V(G)$. For $\mathcal{N} \in (0, \infty]$, we have*

$$\mathcal{K}_{G,x}^{nor}(\infty) \leq \frac{1}{2d_x}\sum_{y\in S_1(x)}\frac{4+\#_\Delta(x,y)}{d_y} - \frac{2}{\mathcal{N}} = \frac{1}{2d_x}\sum_{y\in S_1(x)}\frac{3+d_y-d_y^+}{d_y} - \frac{2}{\mathcal{N}}.$$

Proof. This can be shown by applying Sylvester's criterion to the submatrix of

$$\Gamma_2^{nor}(x) - \frac{1}{\mathcal{N}}(\Delta^{nor}(x))^\top\Delta^{nor}(x) - \mathcal{K}_{G,x}^{nor}(\mathcal{N})\Gamma(x)$$

corresponding to the vertices $\{x\} \sqcup S_2(x)$. □

Finally, we present an example for which $\mathcal{K}_{G,x}^{nor}(\infty)$ and $\mathcal{K}_{G,x}(\infty)$ have different sign at every vertex x. The Figures 7 and 8 are taken from the web-application for calculation of curvature on graphs by David Cushing and George W. Stagg. The number of each vertex is the corresponding curvature values.

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http://teggers.eu/graph/

for calculation of Bakry-Émery curvature $CD(K,\infty)$ on graphs. We also like to thank Anna Felikson for helpful discussions about Coxeter groups, and Boba Hua and Jim Portegies for raising the question whether curvature functions are concave.

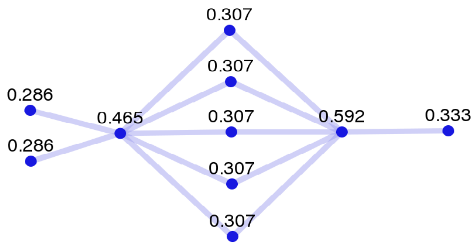

FIGURE 7. Normalized curvature $\mathcal{K}_{G,\cdot}^{nor}(\infty)$

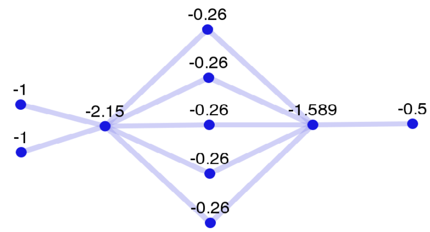

FIGURE 8. Non-normalized curvature $\mathcal{K}_{G,\cdot}(\infty)$

REFERENCES

[1] N. Alon and Y. Roichman, Random Cayley graphs and expanders, Random Structures Algorithms 5 (1994), no. 2, 271-284.

[2] D. Bakry, Functional inequalities for Markov semigroups, Probability measures on groups: recent directions and trends, 91-147, Tata Inst. Fund. Res., Mumbai, 2006.

[3] D. Bakry and M. Émery, Diffusions hypercontractives (French) [Hypercontractive diffusions], Séminaire de probabilités, XIX, 1983/84, Lecture Notes in Math. 1123, J. Azéma and M. Yor (Editors), Springer, Berlin, 1985, pp. 177-206.

[4] W. Ballmann and J. Światkowski, On L^2-cohomology and property (T) for automorphism groups of polyhedral cell complexes, Geom. Funct. Anal. 7 (1997), no. 4, 615-645.

[5] F. Bauer, P. Horn, Y. Lin, G. Lippner, D. Mangoubi, S.-T. Yau, Li-Yau inequality on graphs, J. Differential Geom. 99 (2015), no. 3, pp. 359-405.

[6] B. B. Bhattacharya and S. Mukherjee, Exact and asymptotic results on coarse Ricci curvature of graphs, Discrete Math. 338 (2015), no. 1, 23-42.

[7] A. E. Brouwer and W. H. Haemers, Spectra of graphs, Universitext, Springer, New York, 2012.

[8] P. J. Cameron and J. H. van Lint, Graph theory, coding theory and block designs, London Mathematical Society Lecture Note Series, No. 19, Cambridge University Press, Cambridge-New York-Melbourne, 1975.

[9] D. I. Cartwright, A. M. Mantero, T. Steger, A. Zappa, Groups acting simply transitively on the vertices of a building of type $\tilde{A}_2$. I, Geom. Dedicata 47 (1993), no. 2, 143-166.

[10] F. R. K. Chung, Y. Lin, S.-T. Yau, Harnack inequalities for graphs with non-negative Ricci curvature, J. Math. Anal. Appl. 415 (2014), pp. 25-32.

[11] F. R. K. Chung and S.-T. Yau, Logarithmic Harnack inequalities, Math. Res. Lett. 3 (1996), no. 6, 793-812.

[12] M. W. Davis, The geometry and topology of Coxeter groups, London Mathematical Society Monographs Series, 32, Princeton University Press, Princeton, NJ, 2008.

[13] M. Edjvet and J. Howie, Star graphs, projective planes and free subgroups in small cancellation groups, Proc. London Math. Soc. (3) 57 (1988), no. 2, 301-328.

[14] J. Friedman, R. Murty and J.-P. Tillich, Spectral estimates for abelian Cayley graphs, J. Combin. Theory Ser. B 96 (2006), no. 1, 111-121.

[15] C. Godsil and G. Royle, Algebraic graph theory, Graduate Texts in Mathematics, 207, Springer-Verlag, New York, 2001.

[16] F. Harary, Graph theory, Addison-Wesley Publishing Co., Reading, Mass.-Menlo Park, Calif.-London, 1969.

[17] P. Horn, Y. Lin, S. Liu, S.-T. Yau, Volume doubling, Poincaré inequality and Gaussian heat kernel estimate for nonnegative curvature graphs, arXiv:1411.5087.

[18] B. Hua, Y. Lin, Stochastic completeness for graphs with curvature dimension conditions, Adv. Math. 306 (2017), 279-302.

[19] B. Hua, Y. Lin, Graphs with large girth and nonnegative curvature dimension condition, arXiv:1608.07000.

[20] J. Jost and S. Liu, Ollivier's Ricci curvature, local clustering and curvature-dimension inequalities on graphs, Discrete Comput. Geom. 51 (2014), no. 2, 300-322.

[21] B. Klartag, G. Kozma, P. Ralli, and P. Tetali, Discrete curvature and abelian groups, Canad. J. Math. 68 (2016), 655-674.
[22] A. V. Kolesnikov and E. Milman, Poincaré and Brunn-Minkowski inequalities on weighted Riemannian manifolds with boundary, arXiv:1310.2526.
[23] A. Lakzian and Z. McGuirk, Global Poincaré inequality on graphs via Conical Curvature-Dimension conditions, arXiv:1605.05432.
[24] Y. Lin, L. Lu, and S.-T. Yau, Ricci curvature of graphs, Tohoku Math. J. (2) 63 (2011), no. 4, 605-627.
[25] Y. Lin and S.-T. Yau, Ricci curvature and eigenvalue estimate on locally finite graphs, Math. Res. Lett. 17 (2010), no. 2, 343-356.
[26] S. Liu, F. Münch, and N. Peyerimhoff, Curvature and higher order Buser inequalities for the graph connection Laplacian, arXiv:1512.08134.
[27] S. Liu, F. Münch, and N. Peyerimhoff, Bakry-Emery curvature and diameter bounds on graphs arXiv:1608.07778.
[28] S. Liu and N. Peyerimhoff, Eigenvalue ratios of nonnegatively curved graphs, arXiv:1406.6617.
[29] A. Lubotzky, Discrete groups, expanding graphs and invariant measures, Modern Birkhäuser Classics, Birkhäuser Verlag, Basel, 2010.
[30] F. Münch, Li-Yau inequality on finite graphs via non-linear curvature dimension conditions, arXiv:1412.3340.
[31] F. Münch, Remarks on curvature dimension conditions on graphs, Calc. Var. Partial Differential Equations 56 (2017), no. 1, Art. 11, 8 pp.
[32] S. Ohta, (K,N)-convexity and the curvature-dimension condition for negative N, J. Geom. Anal. 26 (2016), no. 3, 2067-2096.
[33] N. Peyerimhoff and A. Vdovina, Cayley graph expanders and groups of finite width, J. Pure Appl. Algebra 215 (2011), no. 11, 2780-2788.
[34] Z. Qian, Estimates for weighted volumes and applications, Quart. J. Math. Oxford Ser. (2) 48 (1997), no. 190, 235-242.
[35] M. Schmuckenschläger, Curvature of nonlocal Markov generators, in Convex geometric analysis (Berkeley, CA, 1996), Math. Sci. Res. Inst. Publ., 34, K. Ball and V. Milman, ed., Cambridge Univ. Press, Cambridge, 1999, pp. 189-197.
[36] J. J. Seidel, Strongly regular graphs with $(-1,1,0)$ adjacency matrix having eigenvalue 3, Linear Algebra Appl. 1 (1968), 281-298.
[37] J. D. H. Smith, Ricci curvature, circulants, and a matching condition, Discrete Math. 329 (2014), 88-98.

Department of Mathematical Sciences, Durham University, South Road, Durham, DH1 3LE, United Kingdom
E-mail address: `david.cushing@durham.ac.uk`

School of Mathematical Sciences, University of Science and Technology of China, 96 Jinzhai Road, Hefei 230026, Anhui Province, China
E-mail address: `spliu@ustc.edu.cn`

Department of Mathematical Sciences, Durham University, South Road, Durham, DH1 3LE, United Kingdom
E-mail address: `norbert.peyerimhoff@durham.ac.uk`