QUARTIC GRAPHS WHICH ARE BAKRY-ÉMERY CURVATURE SHARP

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ABSTRACT. We give a classification of all connected quartic graphs which are (infinity) curvature sharp in all vertices with respect to Bakry-Émery curvature. The result is based on a computer classification by F. Gurr and L. Watson May and a combinatorial case by case investigation.

1. INTRODUCTION

Curvature is a fundamental notion in geometry which goes back to Gauss and Riemann and was originally defined in the smooth setting of Riemannian manifolds. A challenging problem is to find meaningful curvature notions in discrete settings like graphs and networks.

In this paper we focus on a specific curvature notion on a graph $G = (V, E)$ with a vertex set V and an edge set E, called Bakry-Émery curvature (at dimension $n = \infty$). This curvature notion is based on Bakry-Émery's Γ-calculus and a curvature dimension inequality [BE85], and it was first used by Schmuckenschläger [Schm99] in 1999. The crucial ingredient to define this curvature is a natural notion of a Laplacian. In this paper, we choose the *non-normalized* graph Laplacian Δ, defined on functions $f : V \to \mathbb{R}$ by

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

Bakry-Émery curvature is then a real valued function $\mathcal{K}_\infty(x)$ of the vertices $x \in V$, where the value $\mathcal{K}_\infty(x)$ is fully determined by the combinatorial structure of the (incomplete) 2-ball around x. The precise definition of $\mathcal{K}_\infty(x)$ is given in Subsection 2.1. For readers interested in more details about this curvature notion, see, e.g. [CLP17] and the references therein. Corollary 3.3 of [CLP17] gives the following upper bound of $\mathcal{K}_\infty(x)$ for a D-regular graph:

$$\mathcal{K}_\infty(x) \le 2 + \frac{\#_\Delta(x)}{D},$$

where $\#_\Delta(x)$ is the number of triangles containing x as a vertex. We call a vertex x *(infinity) curvature sharp* if this estimate holds with equality.

The main result in the paper is a complete classification of all 4-regular (quartic) curvature sharp graphs. Before stating our result, let us briefly discuss the classification of 2-regular and 3-regular (cubic) curvature sharp graphs. Cycles C_n, $n \geq 3$, are the only finite connected 2-regular graphs. Since $\mathcal{K}_\infty(C_3) \equiv 2.5$, $\mathcal{K}_\infty(C_4) \equiv 2$ and $\mathcal{K}_\infty(C_n) \equiv 0$ for $n \geq 5$ (see [CLP17, Example 5.20]), C_3 and C_4 are the only 2-regular curvature sharp graphs. For cubic graphs, the only finite connected graphs with positive curvature are K_4, $K_{3,3}$, $K_3 \times K_2$ and the cube $Q^3 = {K_2}^3$ (see Remark at the end of Section 4 in [CKLLS17]). From [CLP17, Examples 5.17, 5.18 and Theorem 7.9], we derive $\mathcal{K}_\infty(K_4) \equiv 3$, $\mathcal{K}_\infty(K_{3,3}) \equiv 2$, $\mathcal{K}_\infty(K_3 \times K_2) \equiv 2$, $\mathcal{K}_\infty(Q^3) \equiv 2$, which implies that K_4, $K_{3,3}$ and Q^3 are the only cubic curvature sharp graphs.

Theorem 1.1. *Let $G = (V, E)$ be a connected quartic graph which is Bakry-Émery curvature sharp in all vertices. Then G is one of the following:*

(i) *The complete graph K_5 with $|V| = 5$, $\mathcal{K}_\infty = 3.5$, $\operatorname{diam} G = 1$;*
(ii) *The octahedral graph O with $|V| = 6$, $\mathcal{K}_\infty = 3$, $\operatorname{diam} G = 2$;*
(iii) *The Cartesian product $K_3 \times K_3$ of two copies of the complete graph K_3 with $|V| = 9$, $\mathcal{K}_\infty = 2.5$, $\operatorname{diam} G = 2$;*
(iv) *The complete bipartite graph $K_{4,4}$ with $|V| = 8$, $\mathcal{K}_\infty = 2$, $\operatorname{diam} G = 2$;*
(v) *The crown graph $C(10)$ with $|V| = 10$, $\mathcal{K}_\infty = 2$, $\operatorname{diam} G = 3$;*
(vi) *The Cayley graph $Cay(D_{12}, S)$ of the dihedral group D_{12} of order 12 with generators $S = \{r^3, s, sr^2, sr^4\}$ with $|V| = 12$, $\mathcal{K}_\infty = 2$, $\operatorname{diam} G = 3$;*
(vii) *The Cayley graph $Cay(D_{14}, S)$ of the dihedral group D_{14} of order 14 with generators $S = \{s, sr, sr^4, sr^6\}$ with $|V| = 14$, $\mathcal{K}_\infty = 2$, $\operatorname{diam} G = 3$;*
(viii) *The 4-dimensional hypercube Q^4 with $|V| = 16$, $\mathcal{K}_\infty = 2$, $\operatorname{diam} G = 4$.*

The proof of this result is based on a computer classification of all quartic incomplete 2-balls with non-negative curvature at their centres. This local classification result was obtained in a 2018 LMS[1] Undergraduate Research Bursary by the last author. The revelant local results of this research can be found in [GW18] and are summarized in Section 2.3 below. They are crucial for the combinatorial arguments given in Section 3 to derive the global classification result. In fact, the proof of Theorem 1.1 is a combinatorial case by case investigation starting with an incomplete 2-ball with a curvature sharp center and extending it to derive a contradiction or to end up with one of the graphs in the above classification.

[1]London Mathematical Society

It is conceivable that the results in [GW18] may also have other applications, for example with regards to the following conjecture about expander graph families (Conjecture 9.11 in [CLP17]):

Conjecture. *Let $D \in \mathbb{N}$ be fixed. Then there do* **not** *exist increasing D-regular expander graphs $\{G_k\}_{k\in\mathbb{N}}$ which are non-negatively curved in all vertices.*

In the case of cubic graphs, it was shown in [CKLLS17, Theorem 1.1] that the only finite connected graphs of non-negative Bakry-Émery curvature are the prism graphs and the Möbius ladders and, therefore, the conjecture is true for $D = 3$. It would be an interesting project to investigate whether the results in [GW18] can be used to verify the conjecture in the case $D = 4$. A full classification of all finite connected non-negatively curved quartic graphs is likely to be out of range due to the large number of local combinatorial possibilities to construct such graphs. However, [GW18] might be useful to derive specific properties contradicting the existence of expander families like, e.g., polynomial volume growth of metric balls.

Let us finish this introduction with an overview about the structure of this paper. In Section 2, we introduce Bakry-Émery curvature and all other relevant notions and present some crucial results needed for the proof of Theorem 1.1. The proof of Theorem 1.1 is given in Section 3.

2. Bakry-Émery curvature

2.1. Motivation of Bakry-Émery curvature.

Readers not familiar with Riemannian manifolds can skip the following explanation and go directly to Definition 2.1 below.

Bakry-Émery curvature is a general (Ricci) curvature notion which can be motivated via the following *curvature-dimension inequality* on an n-dimensional Riemannian manifold $(M, \langle\cdot,\cdot\rangle)$ whose Ricci curvature at x satisfies $\mathrm{Ric}_x(v) \geq K_x|v|^2$ for all tangent vectors $v \in T_xM$:

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

This pointwise inequality holds for all smooth functions f and is a straightforward consequence of *Bochner's formula*, a fundamental fact in Riemannian Geometry (for Bochner's formula see, e.g., [GHL04]). Using Bakry-Émery's Γ-calculus, this inequality can be reformulated as

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

where the symmetric bilinear forms Γ and Γ_2 of two smooth function $f, g : M \to \mathbb{R}$ are defined as

$$2\Gamma(f,g) = \Delta(fg) - f\Delta g - g\Delta f = 2\langle \operatorname{grad} f, \operatorname{grad} g\rangle, \tag{2}$$

$$2\Gamma_2(f,g) = \Delta\Gamma(g,f) - \Gamma(f,\Delta g) - \Gamma(g,\Delta f). \tag{3}$$

Note that Γ and Γ_2 can be defined for any space admitting a reasonable Laplace operator Δ. The idea is to use inequality (1) to define lower Ricci curvature bounds at all points of general spaces admitting Laplace operators. In the case of an arbitrary (not necessarily regular) graph $G = (V, E)$ with vertex set V and edge set E, there is a natural way to introduce a Laplace operator via its adjacency matrix A_G, namely

$$\Delta = A_G - D \cdot \mathrm{Id},$$

where D is a diagonal matrix containing the respective vertex degrees. This operator Δ is called the *non-normalized graph Laplacian* and can also be viewed as a linear operator on the space of functions on the vertices. It is straightforward to see that the Laplacian of a function $f : V \to \mathbb{R}$ is then given by

$$\Delta f(x) = \sum_{y: y\sim x} (f(y) - f(x)), \tag{4}$$

where $y \sim x$ means that the vertices x and y are adjacent.

Note that inequality (1) involves a dimension parameter n, and it is not clear how to choose the dimension for a given graph G. If we do not fix the dimension parameter n, (1) induces a lower Ricci curvature notion at a vertex $x \in V$ *as a function of the dimension.* This viewpoing was taken in [CLP17] and it easy to see that this pointwise curvature function is monotone increasing in n and assumes a finite limit as $n \to \infty$. We refer to the limit as the Bakry-Émery curvature (at infinity) $\mathcal{K}_\infty(x)$ at the vertex x. This limit value can also be directly obtained by dropping the term involving the dimension parameter in (1).

Definition 2.1. *Let $G = (V, E)$ be a graph and Δ be the associated Laplacian defined in* (4). *Let Γ and Γ_2 be the forms defined in* (2) *and* (3). *Then the Bakry-Émery curvature $\mathcal{K}_\infty(x)$ at a vertex x is the supremum of all values $K \in \mathbb{R}$ satisfying*

$$\Gamma_2(f,f)(x) \geq K\Gamma(f,f)(x) \quad \forall f : V \to \mathbb{R}.$$

Moreover, if we have $\mathcal{K}_\infty(x) \geq \mathcal{K}$ at all vertices $x \in V$ for some value $\mathcal{K} \in \mathbb{R}$, we say that G satisfies the (global) curvature-dimension inequality $CD(\mathcal{K}, \infty)$.

A natural class of connected regular graphs satisfying $CD(0, \infty)$ are all abelian Cayley graphs (see [KKRT16] and references therein) and a prominent example with vanishing Bakry-Émery curvature at all vertices is the infinite grid $\mathbb{Z}^n$ with generators $\pm e_j$, $j = 1, \ldots, n$.

2.2. **Fundamental properties of Bakry-Émery curvature.** Before we present some fundamental properties of Bakry-Émery curvature, we need to introduce some relevant notation. All graphs $G = (V, E)$ are assumed to be *connected*, i.e., there is a path between any pair of vertices in V. The degree of a vertex x is denoted by $d_x \in \mathbb{N}$, and a graph G is called D*-regular* if $d_x = D$ for all $x \in V$. The *combinatorial distance* $d(x, y)$ between two vertices $x, y \in V$ is then the length of the shortest path from x to y. The *diameter* of G is defined as

$$\mathrm{diam}(G) = \max_{x,y\in V} d(x, y).$$

Spheres and balls around a vertex $x \in V$ are defined via

$$\begin{aligned} S_k(x) &= \{y \in V \mid d(x, y) = k\}, \\ B_k(x) &= \{y \in V \mid d(x, y) \leq k\}. \end{aligned}$$

The 2-ball $B_2(x)$ has the following decomposition into spheres

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

We call an edge $\{y, z\} \in E$ a *spherical edge* (w.r.t. x) if $d(x, y) = d(x, z)$, and a *radial edge* otherwise. Moreover, the following values associated a reference vertex $x \in V$ are relevant:

$$\begin{aligned} d_x^-(y) &= |\{z \sim y : d(x, y) = d(x, z) + 1\}|, \\ d_x^0(y) &= |\{z \sim y : d(x, y) = d(x, z)\}|, \\ d_x^+(y) &= |\{z \sim y : d(x, y) = d(x, z) - 1\}|, \end{aligned}$$

which we call the *in-degree, spherical degree, out-degree* of y, respectively. Note that $d_y = d_x^-(y) + d_x^0(y) + d_x^+(y)$.

Definition 2.2. *We say that G is S_1-*out regular* at a vertex x, if all the vertices y in $S_1(x)$ have the same out-degree $d_x^+(y)$.*

The *complete 2-ball* around x, denoted by $B_2^{\mathrm{cmp}}(x)$, is the induced subgraph of $B_2(x)$. Furthermore, the *incomplete 2-ball* around x, denoted by $B_2^{\mathrm{inc}}(x)$, is obtained from $B_2^{\mathrm{cmp}}(x)$ with all spherical edges w.r.t. x within $S_2(x)$ being removed. It is important to note that Bakry-Émery curvature $\mathcal{K}_\infty(x)$ at a vertex $x \in V$ is a local value, and it is already determined by the structure of incomplete 2-ball $B_2^{\mathrm{inc}}(x)$. As explained in [CKLLS17, Section 3.4], the explicit calculation of Bakry-Émery curvature at a vertex is a semidefinite programming problem implemented in the interactive curvature calculator which can be found at `http://www.mas.ncl.ac.uk/graph-curvature`. The analytic method for explicit curvature calculation is discussed in Appendix B for the reader's convenience.

In [CLP17], the authors give an upper bound for Bakry-Émery curvature at a vertex in a D-regular graph, and then define the notion of a curvature sharp vertex as follows:

Theorem 2.3. ([CLP17, Corollary 3.3]) *Let $G=(V,E)$ be a D-regular graph. Then Bakry-Émery curvature (of dimension $n=\infty$) at any vertex $x\in V$ satisfies*

$$\mathcal{K}_\infty(x) \le 2 + \frac{\#_\Delta(x)}{D} = 2 + \frac{1}{2D}\sum_{y\in S_1(x)} \#_\Delta(\{x,y\}), \tag{5}$$

where $\#_\Delta(x)$ (resp. $\#_\Delta(e)$) represent the number of triangles containing $x\in V$ (resp. $e\in E$).

Moreover, a vertex $x\in V$ is called (infinity) curvature sharp if (5) *holds with equality.*

From Corollary 5.11 in [CLP17], curvature sharp at x implies S_1-out regularity at x, which means $d_x^+(y)$ is constant for all $y\in S_1(x)$. Equivalently, $\#_\Delta(\{x,y\}) = d_x^0(y) = D-1-d_x^+(y)$ is also constant. Therefore the definition of curvature sharpness at x is equivalent to

$$\mathcal{K}_\infty(x) = 2 + \frac{\#_\Delta(\{x,y\})}{2} \quad \text{for all } y\in S_1(x). \tag{6}$$

Moreover, the following proposition asserts that if curvature sharpness is assumed at all vertices, then the graph has constant curvature.

Proposition 2.4. *Let $G=(V,E)$ be a connected D-regular graph which is curvature sharp at all vertices $x\in V$. Then the number $\#_\Delta(e)$ is constant for all $e\in E$ and G has constant curvature $\mathcal{K}_\infty$.*

Proof. In view of (6), curvature sharpness at y implies $\#_\Delta(\{x,y\}) = \#_\Delta(\{y,z\})$ for any two incident edges $x\sim y$ and $y\sim z$. Curvature sharpness at all vertices then extends the equality $\#_\Delta(\{x,y\}) = \#_\Delta(\{x',y'\})$ for any pair of edges in G (due to connectedness). Therefore, $\#_\Delta(e)$ is constant for all edges $e\in E$, and from equation (6), the curvature $\mathcal{K}_\infty(x) = 2+\frac{\#_\Delta(e)}{2}$ is also constant for all $x\in V$. □

Finally, we need the following *combinatorial analogue* of the classical Bonnet-Myers theorem from Riemannian Geometry (see, e.g., [GHL04]) and its associated rigidity result by Cheng [Ch75].

Theorem 2.5. ([LMP17, Proposition 1.3 and Theorem 1.4]) *Let $G=(V,E)$ be a connected D-regular graph with $K := \inf_{x\in V}\mathcal{K}_\infty(x) > 0$. Then G satisfies Bonnet-Myers' diameter bound*

$$\mathrm{diam}(G) \le \frac{2D}{K},$$

which holds with equality if and only if G is a D-dimensional hypercube.

2.3. **Incomplete 2-balls with non-negative curvature at centers.** In this subsection, we survey the relevant computational results about Bakry-Émery curvature from [GW18]. They are based on a computer program in Python written by the last author during a 2018 LMS Undergraduate Research Bursary.

Firstly, we explain the representations of 2-balls in quartic graphs that were used for these calculations. We fix a vertex v_0 and $S_1(v_0) = \{v_1, v_2, v_3, v_4\}$ (since in a quartic graph, v_0 has four neighbors). The vertices of the 2-sphere are labeled as follows: $S_2(v_0) = \{v_5, v_6, ..., v_m\}$. Then a 2-ball $B_2(v_0)$ centered at v_0 is represented by a list of 3 lists: $B_2(v_0) = [list_1, list_2, list_3]$. The first list determines the S_1 structure (i.e., how the vertices in S_1 are connected to each other) by $list_1 = [a_{12}, a_{13}, a_{14}, a_{23}, a_{24}, a_{34}]$ where each $a_{ij} \in \{0, 1\}$ is a Boolean indicator whether vertices v_i and v_j are adjacent or not. The second list $list_2 = [a_5, a_6, ..., a_m]$ describes the S_1-S_2 structure (i.e., which vertices in S_2 are adjacent to vertices in S_1). For instance, $a_5 = [123]$ means that the vertex v_5 is adjacent to v_1, v_2, v_3 but not to v_4. Lastly, the list $list_3$ describes the S_2 structure (i.e., how the vertices in S_2 are connected to each other). For example, $list_3 = [[57], [58], [68]]$ means that $v_5 \sim v_7$, $v_5 \sim v_8$, and $v_6 \sim v_8$. However, the computation of Bakry-Émery curvature only requires the information of incomplete 2-balls where no spherical edge of $S_2(v_0)$ is present, in which case $list_3 = [\,]$. We refer to *quartic incomplete 2-balls* as those which are incomplete 2-balls of some quartic graph, i.e., every quartic $B_2^{\mathrm{inc}}(v_0)$ has $d_{v_0} = d_{v_1} = ... = d_{v_4} = 4$ and $d_{v_5}, ..., d_{v_m} \leq 4$.

For example, the incomplete 2-ball $B_2^{\mathrm{inc}}(v_0)$ in Figure 1 has the following representation:

$$B_2^{\mathrm{inc}}(v_0) = \Big[\underbrace{[0,1,0,0,1,0]}_{S_1 \text{ structure}},\ \underbrace{[[13],[13],[24],[2],[4]]}_{S_1\text{-}S_2 \text{ structure}},\ [\,] \Big]$$

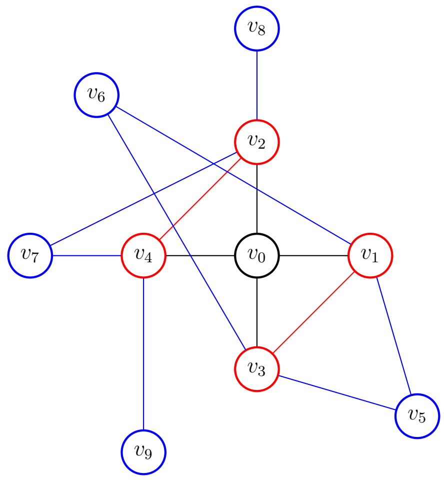

FIGURE 1. $B_2^{\mathrm{inc}}(v_0) = \Big[[0,1,0,0,1,0], [[13],[13],[24],[2],[4]], [\,] \Big]$

Concerning the S_1 structures, we will only consider the 11 *standard* representations (given in the second column of Table 1) since all other S_1 structures can be obtained from them via permutations of the vertices v_1, v_2, v_3, v_4.

The aim of the computer program is to find all non-isomorphic quartic incomplete 2-balls (see Appendix A) and to identify those with particular curvature properties (non-negative curvature and curvature sharpness). The computational results are presented in the following two propositions below. The first proposition gives the number of all non-isomorphic quartic incomplete 2-balls as well as the ones with non-negative curvature at their center. The second proposition gives a list of all 22 quartic incomplete 2-balls that are curvature sharp at their center.

Proposition 2.6. *There are 365 non-isomorphic quartic incomplete 2-balls $B_2^{\mathrm{inc}}(v_0)$. Among them, there are 204 quartic incomplete 2-balls that have non-negative curvature $\mathcal{K}_\infty(v_0)$. For more details, see Table 1.*

Index	Standard S_1 structure	S_1-out regular	Number of incomplete 2-balls	Number of incomplete 2-balls with $\mathcal{K}_\infty(v_0) \geq 0$
1	[0, 0, 0, 0, 0, 0]	True	93	46
2	[1, 0, 0, 0, 0, 0]	False	120	55
3	[1, 0, 0, 0, 0, 1]	True	40	24
4	[1, 1, 0, 0, 0, 0]	False	55	31
5	[1, 1, 1, 0, 0, 0]	False	8	8
6	[1, 1, 0, 1, 0, 0]	False	10	4
7	[1, 1, 0, 0, 1, 0]	False	24	21
8	[1, 1, 0, 0, 1, 1]	True	7	7
9	[1, 1, 1, 1, 0, 0]	False	5	5
10	[1, 1, 1, 1, 1, 0]	False	2	2
11	[1, 1, 1, 1, 1, 1]	True	1	1
Total			365	204

Table 1. Number of incomplete 2-balls classified by their standard S_1 structure

In fact the above result is not used in our proof in Section 3. The following result, however, is crucial for the proof:

Proposition 2.7. *There are 22 non-isomorphic quartic incomplete 2-balls $B_2^{\mathrm{inc}}(v_0)$ which are curvature sharp in v_0. They are listed in Table 2.*

$\#_\Delta(e)$, $v_0 \in e \in E$	Incomplete 2-ball $B_2^{\mathrm{inc}}(v_0)$			$\mathcal{K}_\infty(v_0)$
	Index	S_1 structure	S_1-S_2 structure	
3	1.1	[1, 1, 1, 1, 1, 1]	$\emptyset$	3.5
2	2.1	[1, 1, 0, 0, 1, 1]	[1234]	3.0
	2.2	[1, 1, 0, 0, 1, 1]	[123], [4]	
	2.3	[1, 1, 0, 0, 1, 1]	[12], [3], [4]	
	2.4	[1, 1, 0, 0, 1, 1]	[14], [2], [3]	
	2.5	[1, 1, 0, 0, 1, 1]	[1], [2], [3], [4]	
	2.6	[1, 1, 0, 0, 1, 1]	[12], [34]	
	2.7	[1, 1, 0, 0, 1, 1]	[14], [23]	
1	3.1	[1, 0, 0, 0, 0, 1]	[1234], [13], [24]	2.5
	3.2	[1, 0, 0, 0, 0, 1]	[13], [13], [24], [24]	
	3.3	[1, 0, 0, 0, 0, 1]	[13], [14], [23], [24]	
	3.4	[1, 0, 0, 0, 0, 1]	[1234], [1234]	
0	4.1	[0, 0, 0, 0, 0, 0]	[1234], [1234], [1], [2], [3], [4]	2.0
	4.2	[0, 0, 0, 0, 0, 0]	[1234], [1234], [12], [3], [4]	
	4.3	[0, 0, 0, 0, 0, 0]	[1234], [1234], [123], [4]	
	4.4	[0, 0, 0, 0, 0, 0]	[1234], [12], [13], [24], [34]	
	4.5	[0, 0, 0, 0, 0, 0]	[12], [13], [14], [23], [24], [34]	
	4.6	[0, 0, 0, 0, 0, 0]	[123], [123], [14], [24], [34]	
	4.7	[0, 0, 0, 0, 0, 0]	[1234], [1234], [12], [34]	
	4.8	[0, 0, 0, 0, 0, 0]	[1234], [123], [124], [34]	
	4.9	[0, 0, 0, 0, 0, 0]	[123], [124], [134], [234]	
	4.10	[0, 0, 0, 0, 0, 0]	[1234], [1234], [1234]	

TABLE 2. Incomplete 2-ball structures with a curvature sharp center, i.e. $\mathcal{K}_\infty(v_0) = 2 + \frac{\#_\Delta(e)}{2}$

3. Proof of the classification theorem

Proof of Theorem 1.1. Let us start with a reference vertex v_0 and $S_1(v_0) = \{v_1, v_2, v_3, v_4\}$. We will perform a case-by-case analysis of all 22 possible (non-isomorphic) $B_2^{\mathrm{inc}}(v_0)$-structures which are curvature sharp at v_0, provided in Table 2.

Since we assume all vertices v to be curvature sharp, any incomplete 2-ball $B_2^{\mathrm{inc}}(v)$ must be one of the 22 possible types, but their types can differ from vertex to vertex. However, we will see a posteriori that each globally curvature sharp graph generated by these cases is vertex transitive and, therefore, the incomplete 2-ball types of all its vertices coincide.

Moreover, Proposition 2.4 asserts that for every edge $e \in E$ the number of triangles containing e, $\#_\Delta(e)$, is uniform. We will therefore use the number $\#_\Delta(e) \in \{0, 1, 2, 3\}$ for our case separation. Table 3 provides an overview about all incomplete 2-ball structures that lead to globally curvature sharp graphs.

3.1. **Case $\#_\Delta(e) = 3$ or $\#_\Delta(e) = 2$.** In the case $\#_\Delta(e) = 3$, the S_1 structure immediately implies that G is the complete graph K_5.

$\#_\Delta(e)$, $v_0 \in e \in E$	Incomplete 2-ball $B_2^{\text{inc}}(v_0)$			resulting graph(s)
	Index	S_1 structure	S_1-S_2 structure	
3	1.1	[1, 1, 1, 1, 1, 1]	$\emptyset$	K_5
2	2.1	[1, 1, 0, 0, 1, 1]	[1234]	O
1	3.3	[1, 0, 0, 0, 0, 1]	[13], [14], [23], [24]	$K_3 \times K_3$
0	4.5	[0, 0, 0, 0, 0, 0]	[12], [13], [14], [23], [24], [34]	$Cay(D_{14}, S)$ and Q^4
	4.6	[0, 0, 0, 0, 0, 0]	[123], [123], [14], [24], [34]	$Cay(D_{12}, S)$
	4.9	[0, 0, 0, 0, 0, 0]	[123], [124], [134], [234]	$C(10)$
	4.10	[0, 0, 0, 0, 0, 0]	[1234], [1234], [1234]	$K_{4,4}$

TABLE 3. Incomplete 2-ball structures leading to globally curvature sharp graphs

Next we deal with the case $\#_\Delta(e) = 2$. If $B_2^{\text{inc}}(v_0)$ is of type 2.1, then G is immediately the Octahedral graph O. Otherwise, if $B_2^{\text{inc}}(v_0)$ is of type 2.2, 2.3, 2.4, 2.5, 2.6 or 2.7, the S_1-S_2 structure infers that v_2 and v_4 have no common neighbor in $S_2(v_0)$. Thus we have $\#_\Delta(\{v_2, v_4\}) = 1$, namely the triangle $\{v_0v_2v_4\}$; contradiction to $\#_\Delta(e) = 2$.

3.2. **Case $\#_\Delta(e) = 1$.** In the case $\#_\Delta(e) = 1$, we will show that the incomplete 2-ball $B_2^{\text{inc}}(v_0)$ has only one possible structure, which is of type 3.3. Moreover, it leads to a unique graph G, namely the Cartesian product $K_3 \times K_3$.

3.2.1. **Case $B_2^{\text{inc}}(v_0)$ is of type 3.1.** Denote $v_5, v_6, v_7 \in S_2(v_0)$ with the patterns

$$v_5 \equiv [1234] \qquad v_6 \equiv [13] \qquad v_7 \equiv [24].$$

Then $\{v_0v_1v_2\}$ and $\{v_1v_2v_5\}$ are triangles, so $\#_\Delta(\{v_1, v_2\}) \geq 2$; contradiction.

We purposedly use "$\equiv$" to describe the pattern of a vertex in a 2-sphere to allow the possibility that two vertices may have the same pattern e.g., $v_5 \equiv v_6 \equiv [13]$ even though $v_5 \neq v_6$.

3.2.2. **Case $B_2^{\text{inc}}(v_0)$ is of type 3.2.** Denote $v_5, v_6, v_7, v_8 \in S_2(v_0)$ with the patterns

$$v_5 \equiv v_6 \equiv [13] \qquad v_7 \equiv v_8 \equiv [24].$$

Note that v_1 has four neighbors v_0, v_2, v_5, v_6. Since v_5 is not a neighbor of v_0 and v_2, the fact that $\#_\Delta(\{v_1, v_5\}) = 1$ implies that v_5 is a neighbor of v_6. Now $\{v_1v_5v_6\}$ and $\{v_3v_5v_6\}$ are triangles, so $\#_\Delta(\{v_5, v_6\}) \geq 2$; contradiction.

3.2.3. **Case $B_2^{\text{inc}}(v_0)$ is of type 3.4.** Denote $v_5, v_6 \in S_2(v_0)$ with the patterns $v_5 \equiv v_6 \equiv [1234]$. Then $\{v_0v_1v_2\}$, $\{v_1v_2v_5\}$, and $\{v_1v_2v_6\}$ are triangles, so $\#_\Delta(\{v_1, v_2\}) = 3$; contradiction.

3.2.4. **Case $B_2^{\mathrm{inc}}(v_0)$ is of type 3.3.** Denote $v_5, v_6, v_7, v_8 \in S_2(v_0)$ with the patterns

$$v_5 \equiv [13] \quad v_6 \equiv [14] \quad v_7 \equiv [23] \quad v_8 \equiv [24].$$

Consider v_1 as a center with four neighbors v_0, v_2, v_5, v_6. Since $v_5 \not\sim v_0$ and $v_5 \not\sim v_2$, the fact that $\#_\Delta(\{v_1, v_5\}) = 1$ implies $v_5 \sim v_6$. Similarly, by centering at v_2, $\#_\Delta(\{v_2, v_7\}) = 1$ implies $v_7 \sim v_8$.
By centering at v_3, $\#_\Delta(\{v_3, v_5\}) = 1$ implies $v_5 \sim v_7$.
By centering at v_4, $\#_\Delta(\{v_4, v_6\}) = 1$ implies $v_6 \sim v_8$.

Now $B_2^{\mathrm{inc}}(v_0)$ with additional edges $v_5 \sim v_6 \sim v_8 \sim v_7 \sim v_5$ results in a quartic graph, which is in fact the Cartesian product $K_3 \times K_3$ (see Figure 2).

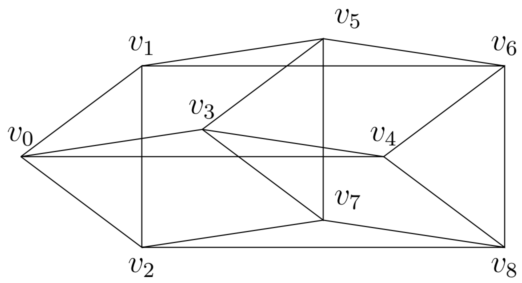

FIGURE 2. Cartesian product $K_3 \times K_3$

3.3. **Case $\#_\Delta(e) = 0$.** Lastly, we deal with the most difficult case where $\#_\Delta(e) = 0$ (i.e. G is triangle-free) and we expect to derive 5 possibilities of G, depending on its incomplete 2-ball structure. Henceforth, we restrict ourselves to the "bottom half" of Table 2, that is the ones indexed by 4.1-4.10.

From now on, we introduce a new notation for S_1-S_2 structure of the 2-ball $B_2^{\mathrm{inc}}(v_i)$, which is centered around the vertex v_i (for $i \in \{1, 2, 3, 4\}$). To do so, we add a subscript i to the pattern of each vertex on the two-sphere $S_2(v_i)$.

For example, assuming v_1 has the neighbors v_0, v_5, v_6, v_7, the subscripts 1 in the following patterns

$$v_2 \equiv [0567]_1 \qquad v_3 \equiv [0567]_1 \qquad v_4 \equiv [056]_1$$

signifies that they describe vertices in the S_1-S_2 structure of $B_2^{\mathrm{inc}}(v_1)$.

Moreover, as in previous arguments, patterns are written without subscripts when we describe the S_1-S_2 structure of $B_2^{\mathrm{inc}}(v_0)$.

3.3.1. **Case $B_2^{\mathrm{inc}}(v_0)$ is of type 4.10.** It is straightforward to deduce that G is the complete bipartite graph $K_{4,4}$.

3.3.2. **Case $B_2^{\rm inc}(v_0)$ is of type 4.1, 4.2, 4.3, or 4.7.** Note that all these cases have precisely two vertices in $S_2(v_0)$ with the patterns [1234]. Let us denote them by v_5 and v_6.

Consider v_1 as a center with three known neighbors v_0, v_5, v_6, and the other unknown neighbor, which we denote by v_7. Now v_2, v_3, v_4 are in $S_2(v_1)$ and all of them are neighbors of v_0, v_5, v_6, so they will have the following patterns:

$$v_2 \equiv [056{*_2}]_1 \qquad v_3 \equiv [056{*_3}]_1 \qquad v_4 \equiv [056{*_4}]_1 \tag{7}$$

where (for $i \in \{2,3,4\}$) each $*_i$ takes value 7 or "empty", depending on whether v_i is a neighbor of v_7 or not.

When comparing the patterns in (7) to the S_1-S_2 structures in Table 2, we can see that the possible structures of $B_2^{\rm inc}(v_1)$ are of type either 4.3 or 4.10. However, an incomplete 2-ball of type 4.10 previously led to the resulting graph $G = K_{4,4}$. In case $B_2^{\rm inc}(v_1)$ is of type 4.3, two vertices have their patterns $[0567]_1$ and one vertex has its pattern $[056]_1$. Without loss of generality, let the patterns in (7) take values

$$v_2 \equiv [0567]_1 \qquad v_3 \equiv [0567]_1 \qquad v_4 \equiv [056]_1$$

which means $v_4 \not\sim v_7$. Now consider v_4 as a center, with neighbors v_0, v_5, v_6, and another neighbor denoted by $v_8 (\neq v_7)$. Note that due to the S_1 structure of v_0 being $[0,0,0,0,0,0]$, it means that v_4 is not a neighbor of v_1, v_2, v_3. Thus v_1, v_2, v_3 are in $S_2(v_4)$, and all of them are neighbors of v_0, v_5, v_6, v_7 (but not of v_8). Hence, v_1, v_2, v_3 have all the same pattern $[056]_4$, which does not belong to any S_1-S_2 structure in Table 2.

3.3.3. **Case $B_2^{\rm inc}(v_0)$ is of type 4.4.** Denote the vertices on $S_2(v_0)$ by patterns

$$v_5 \equiv [1234] \qquad v_6 \equiv [12] \qquad v_7 \equiv [13] \qquad v_8 \equiv [24] \qquad v_9 \equiv [34].$$

Consider v_1 as a center with four neighbors v_0, v_5, v_6, v_7. Now v_2, v_3, v_4 are in $S_2(v_1)$ with the patterns

$$v_2 \equiv [056]_1 \qquad v_3 \equiv [057]_1 \qquad v_4 \equiv [05]_1,$$

which does not belong to any S_1-S_2 structure in Table 2.

3.3.4. **Case $B_2^{\rm inc}(v_0)$ is of type 4.8.** Denote the vertices on $S_2(v_0)$ by patterns

$$v_5 \equiv [1234] \qquad v_6 \equiv [123] \qquad v_7 \equiv [124] \qquad v_8 \equiv [34].$$

Consider v_3 as a center with four neighbors v_0, v_5, v_6, v_8. Now v_1, v_2, v_4 are in $S_2(v_3)$ with the structure

$$v_1 \equiv [056]_3 \qquad v_2 \equiv [056]_3 \qquad v_4 \equiv [058]_3,$$

which does not belong to any S_1-S_2 structure in Table 2.

3.3.5. **Case $B_2^{\text{inc}}(v_0)$ is of type 4.6.** From now on, instead of calling the vertices on $S_2(v_0)$ as v_5, v_6 and so on, we call them differently by names reflecting their patterns.

In this particular case, we will denote the vertices on $S_2(v_0)$ by patterns

$$v_{123} \equiv v'_{123} \equiv [123] \qquad v_{14} \equiv [14] \qquad v_{24} \equiv [24] \qquad v_{34} \equiv [34].$$

Consider v_1 as a center with four neighbors $v_0, v_{14}, v_{123}, v'_{123}$. Henceforth, we also describe patterns no longer just by the indices of the involved vertices but by the vertices themselves. In this case, the vertices v_2, v_3, v_4 are in $S_2(v_1)$ with patterns

$$v_2 \equiv v_3 \equiv [v_0 v_{123} v'_{123}]_1 \qquad v_4 \equiv [v_0 v_{14}]_1,$$

and according to Table 2, the $B_2^{\text{inc}}(v_1)$ must be of type 4.6. That is, the other two vertices in $S_2(v_1)$, namely A and B, will have patterns

$$A \equiv [v_{123} v_{14}]_1 \qquad B \equiv [v'_{123} v_{14}]_1 \tag{8}$$

In principle, it is possible that A or B could coincide with v_{24} or v_{34}. However, this can be excluded by the following arguments. If $A = v_{24}$, we would have a triangle $\{v_4 v_{14} v_{24}\}$, and if $A = v_{34}$, we would have a triangle $\{v_4 v_{14} v_{34}\}$. The same reasoning applies to $B = v_{24}$ or $B = v_{34}$.

Next, consider v_4 as a center with four neighbors $v_0, v_{14}, v_{24}, v_{34}$. Now v_1, v_2, v_3, A, B are in $S_2(v_4)$ with the patterns

$$v_1 \equiv [v_0 v_{14}]_4 \qquad v_2 \equiv [v_0 v_{24}]_4 \qquad v_3 \equiv [v_0 v_{34}]_4 \qquad A \equiv [v_{14} *]_4 \qquad B \equiv [v_{14} *]_4,$$

where each $*$ represents some unknown vertex/vertices. According to Table 2, the only possible type of $B_2^{\text{inc}}(v_4)$ is 4.6. That is, A and B are in $S_2(v_4)$ with patterns

$$A \equiv B \equiv [v_{14} v_{24} v_{34}]_4. \tag{9}$$

The information (8) and (9) tells us that we have a quartic graph as in Figure 3, which is indeed a Cayley graph of D_{12} (see Figure 7 in Remark 3.1 below).

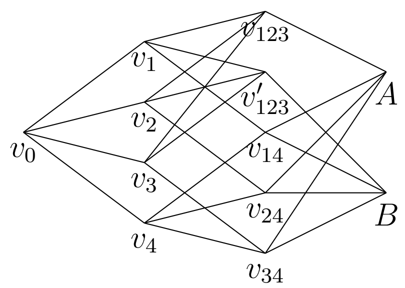

FIGURE 3. The unique graph arising in case $B_2^{\text{inc}}(v_0)$ is of type 4.6

3.3.6. **Case $B_2^{\rm inc}(v_0)$ is of type 4.5.** Denote the vertices on $S_2(v_0)$ by patterns

$$v_{12} \equiv [12] \quad v_{13} \equiv [13] \quad v_{14} \equiv [14] \quad v_{23} \equiv [23] \quad v_{24} \equiv [24] \quad v_{34} \equiv [34].$$

For each $i \in \{1,2,3,4\}$, consider v_i as a center with four neighbors $v_0, v_{ij}, v_{ik}, v_{il}$ where $\{i,j,k,l\} = \{1,2,3,4\}$ (and from now on, $v_{ij} = v_{ji}$ by convention). The vertices v_j, v_k, v_l are then in $S_2(v_i)$ with patterns

$$v_j \equiv [v_0 v_{ij}]_i \qquad v_k \equiv [v_0 v_{ik}]_i \qquad v_l \equiv [v_0 v_{il}]_i.$$

According to Table 2, the type of $B_2^{\rm inc}(v_i)$ must be either 4.5 or 4.6 (and we can safely assume the type 4.5, since we previously dealt with the case where an incomplete 2-ball is of type 4.6).

Since $B_2^{\rm inc}(v_i)$ is of type 4.5, we suppose $S_2(v_i) = \{v_j, v_k, v_l, A^i_{jk}, A^i_{jl}, A^i_{kl}\}$ with patterns

$$\begin{aligned} &v_j \equiv [v_0 v_{ij}]_i \qquad v_k \equiv [v_0 v_{ik}]_i \qquad v_l \equiv [v_0 v_{il}]_i \\ &A^i_{jk} \equiv [v_{ij} v_{ik}]_i \qquad A^i_{jl} \equiv [v_{ij} v_{il}]_i \qquad A^i_{kl} \equiv [v_{ik} v_{il}]_i. \end{aligned} \tag{10}$$

Here, A^i_{jk} and A^i_{kj} represent the same vertex.

Note that none of the vertices $A^i_{jk}, A^i_{jl}, A^i_{kl}$ can coincide with the vertices v_{jk}, v_{jl}, v_{kl}, since this would always lead to the existence of some triangle, namely, $v_s v_{is} v_{st}$ for some distinct $s,t \in \{j,k,l\}$. In conclusion,

$$A^i_{jk}, A^i_{jl}, A^i_{kl} \in S_3(v_0).$$

For every vertex $w \in S_3(v_0)$, we know that

$$w \sim v_{ij} \quad \text{for some distinct } i,j \in \{1,2,3,4\}, \tag{11}$$

and therefore $w \in S_2(v_i) \cap S_2(v_j)$. Since $w \in S_2(v_i)$, (10) implies that w coincides with one of $A^i_{jk}, A^i_{jl}, A^i_{kl}$, so it is adjacent to v_{ij} by (11) and v_{is} for some $s \neq j$.

Similarly, since $w \in S_2(v_j)$, w is also adjacent to v_{ij} and v_{jt} for some $t \neq i$. Therefore, w has at least 3 different neighbors in $S_2(v_0)$, namely v_{ij}, v_{is}, v_{jt}, so its in-degree (w.r.t. v_0) is

$$d^-_{v_0}(w) \geq 3 \qquad \text{for all } w \in S_3(v_0).$$

On the other hand, for every vertex $z \in S_2(v_0)$, its in-degree is $d^-_{v_0}(z) = 2$, so its out-degree is $d^+_{v_0}(z) \leq 2$. Counting edges between $S_2(v_0)$ and $S_3(v_0)$ then gives

$$12 \geq \sum_{z \in S_2(v_0)} d^+_{v_0}(z) = \sum_{w \in S_3(v_0)} d^-_{v_0}(w) \geq 3|S_3(v_0)|, \tag{12}$$

so we have $|S_3(v_0)| \leq 4$. Moreover, since $A^i_{jk}, A^i_{jl}, A^i_{kl} \in S_3(v_0)$, we must have $3 \leq |S_3(v_0)| \leq 4$.

- Case $|S_3(v_0)| = 3$: then we know that $S_3(v_0) = \{A^i_{jk}, A^i_{jl}, A^i_{kl}\}$. Observe also that v_{ij} has four neighbors, namely $S_1(v_{ij}) = \{v_i, v_j, A^i_{jk}, A^i_{jl}\}$.

  Since these arguments hold for all indices i, j, we are allowed to interchange them, that is

$$S_3(v_0) = \{A^i_{jk}, A^i_{jl}, A^i_{kl}\} = \{A^j_{ik}, A^j_{il}, A^j_{kl}\}$$
$$S_1(v_{ij}) = \{v_i, v_j, A^i_{jk}, A^i_{jl}\} = \{v_i, v_j, A^j_{ik}, A^j_{il}\}.$$

  which implies that A^i_{kl} and A^j_{kl} coincide. By definition, it means that this vertex $A^i_{kl} \in S_3(v_0)$ is connected to $v_{ik}, v_{il}, v_{jk}, v_{jl}$, that is

$$S_1(A^i_{kl}) = \{v_{ik}, v_{il}, v_{jk}, v_{jl}\}.$$

  Since this argument holds for all combinations of i, j, k, l, we derive the information about all three vertices $A^1_{23}, A^1_{24}, A^1_{34} \in S_3(v_0)$:

$$S_1(A^1_{23}) = \{v_{12}, v_{13}, v_{24}, v_{34}\},$$
$$S_1(A^1_{24}) = \{v_{12}, v_{14}, v_{23}, v_{34}\},$$
$$S_1(A^1_{34}) = \{v_{13}, v_{14}, v_{23}, v_{24}\},$$

  which results in a quartic graph as in Figure 4, which is indeed a Cayley graph of D_{14} (see Figure 8 in Remark 3.1).

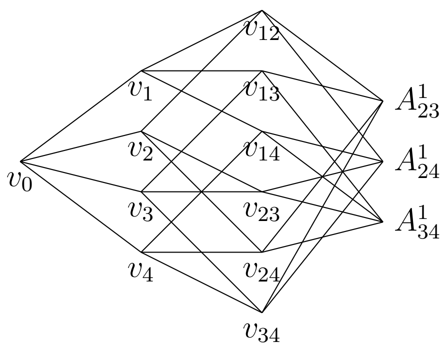

FIGURE 4. The graph arising in case $B_2^{\mathrm{inc}}(v_0)$ is of type 4.6 and $|S_3(v_0)| = 3$

- Case $|S_3(v_0)| = 4$: We claim that in this case our graph G has diameter $\mathrm{diam}(G) \geq 4$. Assume for the sake of contradiction that $\mathrm{diam}(G) = 3$ and the 4-sphere $S_4(v_0)$ is empty.

  Since $|S_3(v_0)| = 4$, the inequality (12) holds with equality, which implies that for all $w \in S_3(v_0)$, the in-degree $d^-_{v_0}(w) = 3$. Thus the spherical degree $d^0_{v_0}(w) = 1$. In particular, each of the vertices $A^1_{23}, A^1_{24}, A^1_{34}$ must be adjacent to another vertex in $S_3(v_0)$. However, note that no pair of vertices $A^1_{23}, A^1_{24}, A^1_{34}$ are adjacent (otherwise, if A^1_{jk} and A^1_{jl} were connected, then they would form a triangle $\Delta v_{1j}A^1_{jk}A^1_{jl}$). Thus $A^1_{23}, A^1_{24}, A^1_{34}$ must be adjacent to the the fourth vertex in $S_3(v_0)$, which we may denote by P. Then the spherical degree $d^0_{v_0}(P) = 3$, contradiction.

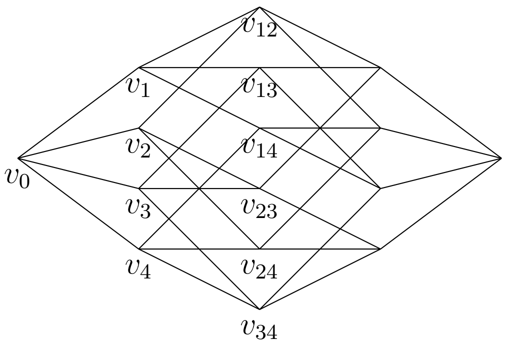

FIGURE 5. The 4-dimensional hypercube Q^4

Therefore we have shown that $\mathrm{diam}(G) \geq 4$. On the other hand, Theorem 2.5 gives the following diameter bound for Bakry-Émery curvature:

$$\mathrm{diam}(G) \leq \frac{2D}{K} = \frac{2 \cdot 4}{2} = 4,$$

as we are working with quartic graphs ($D = 4$) and $K = \inf_x (K)_\infty(x) = 2$ (see Table 2). Since the graph G has diameter $\mathrm{diam}(G) = 4$, it must be the 4-dimensional hypercube Q^4 (as illustrated in Figure 5) by the rigidity statement in Theorem 2.5.

3.3.7. **Case $B_2^{\mathrm{inc}}(v_0)$ is of type 4.9.** Denote the vertices on $S_2(v_0)$ by patterns

$$v_{123} \equiv [123] \qquad v_{124} \equiv [124] \qquad v_{134} \equiv [134] \qquad v_{234} \equiv [234].$$

For any $\{i, j, k, l\} = \{1, 2, 3, 4\}$, each vertex $v_{ijk} \in S_2(v_0)$ has in-degree $d^-_{v_0}(v_{ijk}) = 3$ and spherical-degree $d^0_{v_0}(v_{ijk}) = 0$ (as G is triangle-free), so v_{ijk} must be connected to exactly one vertex on $S_3(v_0)$ (depending on the choice of i, j, k) which we denote by $A_{ijk} \in S_3(v_0)$. Note that these vertices A_{ijk} might coincide (in fact, we will see that they are all the same vertex).

Consider v_i as a center with four neighbors $v_0, v_{ijk}, v_{ijl}, v_{ikl}$. The vertices $v_j, v_k, v_l \in S_2(v_i)$ will have patterns

$$v_j \equiv [v_0 v_{ijk} v_{ijl}]_i \qquad v_k \equiv [v_0 v_{ijk} v_{ikl}]_i \qquad v_l \equiv [v_0 v_{ijl} v_{ikl}]_i.$$

According to Table 2, $B_2^{\mathrm{inc}}(v_i)$ must be of
type 4.9 and, therefore, $|S_2(v_i)| = 4$. We denote the so far unlabeled vertex of $S_2(v_i)$ by A_i and we have $S_2(v_i) = \{v_j, v_k, v_l, A_i\}$ and A_i will

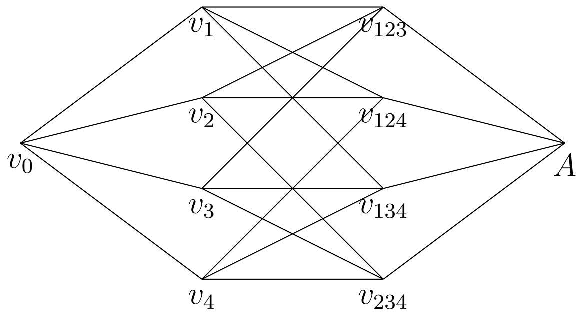

FIGURE 6. The crown graph $C(10)$

have a pattern

$$A_i \equiv [v_{ijk} v_{ijl} v_{ikl}]_i. \tag{13}$$

Since $d(A_i, v_i) = 2$ and $A_j \neq v_j, v_k, v_l$, we have

$$A_i \notin \{v_0, v_i, v_j, v_k, v_{ijk}, v_{ijl}, v_{ikl}\}.$$

We can also rule out $A_i = v_{jkl}$ (for, otherwise, $2 = d(A_i, v_i) = d(v_{jkl}, v_i)$ would imply that $A_i = v_{jkl}$ is adjacent to one of the neighbors $v_{ijk}, v_{ijl}, v_{ikl}$ of v_i; but any edge between two vertices of $v_{ijk}, v_{ijl}, v_{ikl}, v_{jkl}$ would create a triangle and, therefore, a contradiction). These considerations show that $A_i \in S_3(v_0)$ and $A_i \sim v_{ijk}$ by (13). By definition of the vertices A_{ijk}, we conclude that

$$A_i = A_{ijk} \qquad \text{for all permutations } \{i, j, k, l\} = \{1, 2, 3, 4\}.$$

In particular,

$$\begin{aligned} A_1 &= A_{123} = A_{124} = A_{134} \\ A_2 &= A_{123} = A_{124} \qquad\qquad = A_{234}, \end{aligned}$$

which means $A_{123}, ..., A_{234}$ all coincide, and $S_3(v_0)$ has only one vertex. As a result, G is the crown graph $C(10)$, as shown in Figure 6.

After consideration of all possible cases we have now completed our classification result of quartic curvature sharp graphs (8 of them in total). □

Remark 3.1. *Figures 7 and 8 illustrate that the graphs in (vi) and (vii) of Theorem 1.1 have indeed the stated Cayley graph structure.*

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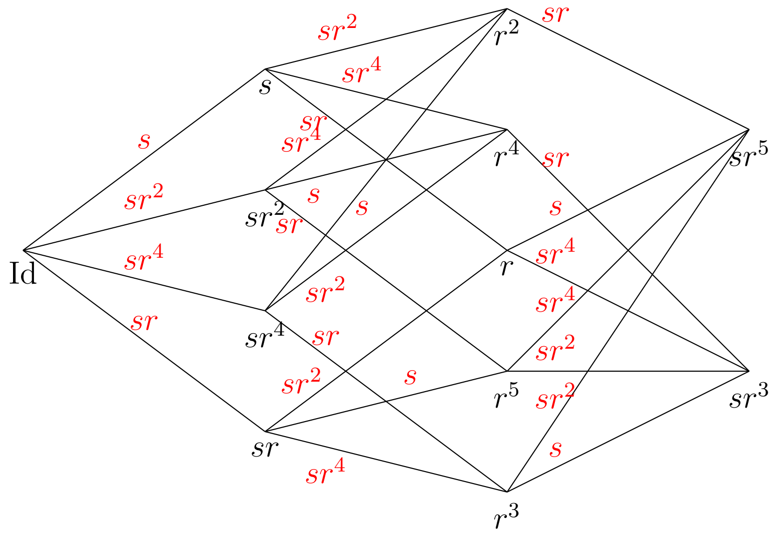

Figure 7. The Cayley graph $Cay(D_{12}, S)$ with $S = \{r^3, s, sr^2, sr^4\}$

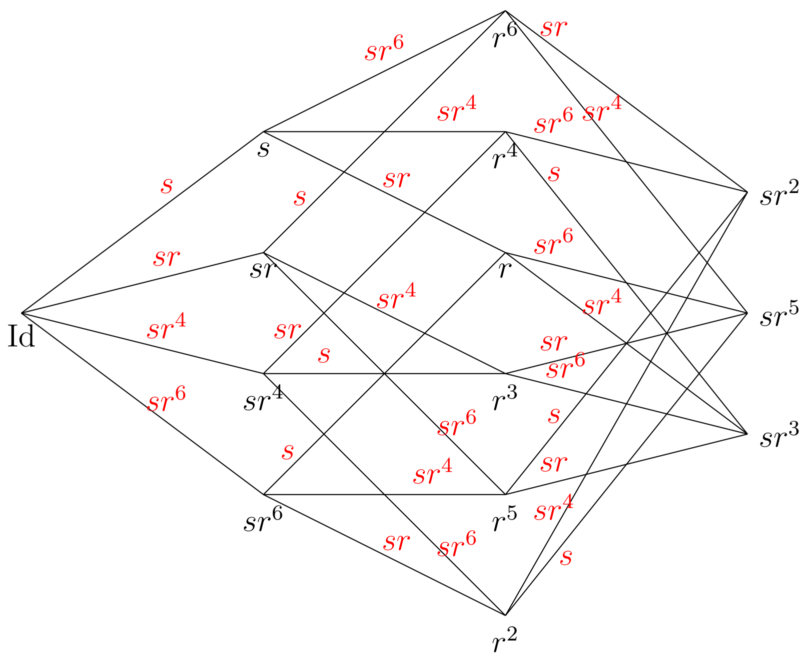

Figure 8. The Cayley graph $Cay(D_{14}, S)$ with $S = \{s, sr, sr^4, sr^6\}$

Appendix A. Alogorithm to generate all quartic incomplete 2-balls

The information in Tables 1 and 2 was derived from the Python code written by Gurr and the last author, see [GW18]. In this appendix we briefly explain the ideas behind this code which generates all non-isomorphic quartic incomplete 2-balls using the three python functions `generate_all_incomp_twoballs`, `generate_special_twoballs`, and `iso`.

Before we discuss these functions in more detail, let us recall our description of an incomplete 2-ball structure $B_2^{\mathrm{inc}}(v_0)$ introduced in Subsection 2.3:

$$\Bigg[\underbrace{[a_{12}, a_{13}, a_{14}, a_{23}, a_{24}, a_{34}]}_{list_1}, \underbrace{[\underbrace{[\cdots]}_{a_5}, \underbrace{[\cdots]}_{a_6}, ..., \underbrace{[\cdots]}_{a_m}]}_{list_2}, \underbrace{[\,]}_{list_3=\emptyset} \Bigg],$$

where

- $list_1$ describes the S_1 structure: each $a_{ij} \in \{0,1\}$ tells whether vertices v_i and v_j are adjacent or not).
- $list_2$ describes the S_1-S_2 structure: for example, $a_5 = [123]$ means that the vertex v_5 is adjacent to v_1, v_2, v_3 but not to v_4.
- $list_3$ provides information about spherical edges in S_2 and is left empty since we only consider "incomplete" 2-balls.

The above incomplete 2-ball representation is called *standardized* if

(1) $list_1$ coincides with one of the 11 standard S_1 structures (see the second column of Table 1), and
(2) $list_2$ is lexicographically ordered (for example, the lexicographic ordering of [[32],[134],[3],[243]] is [[134],[234],[23],[3]]).

A.1. **Function `generate_all_incomp_twoballs`.** This function finds all possible quartic incomplete 2-balls.

First, the function loops through all 11 standard S_1 structures. For each such structure (i.e., fixing $list_1$), the function then finds all possible $list_2$'s.

Each S_1 structure determines an array

$$\texttt{avail\_outdeg} = [d^+_{v_0}(v_1), d^+_{v_0}(v_2), d^+_{v_0}(v_3), d^+_{v_0}(v_4)]$$

of available out-degrees of vertices v_i, $i \in \{1,2,3,4\}$ from the relation $4 = d^+_{v_0}(v_i) + d^0_{v_0}(v_i) + d^-_{v_0}(v_i)$, where the in-degree $d^-_{v_0}(v_i) = 1$ and the spherical degree $d^0_{v_0}(v_i)$ is known from the S_1 structure. A vertex v_i is called *unsaturated* if its available out-degree is more than zero. The available out-degree of a vertex v_i must agree with the total number of appearances of the entry i in $list_2$ in any incomplete 2-ball representation.

Next, the function calculates all *valid* partitions of the total number $n =$ `sum(avail_outdeg)` of available out-degrees. Each partition determines the lengths of brackets of $a_5, a_5, ..., a_m$ in $list_2$. For example, the partition 332 means that a_5, a_6, a_7 are brackets of length $3, 3, 2$, respectively.

A partition is called *valid* if it satisfies the following two conditions:

(1) Each number in the partition must not exceed the number of unsaturated vertices in $S_1(v_0)$.
(2) The length of the partition is at least `max(avail_outdeg)`.

For example, starting with the S_1 structure $list_1 = [1, 0, 0, 0, 0, 1]$, we have `avail_outdeg`$= [2, 2, 2, 2]$, and the valid partitions of $n = 8$ are given by

$$44, 431, 422, 4211, 41111, 332, 3311, 3221, 32111, 311111,$$
$$222, 22211, 221111, 2111111, 11111111.$$

After calculating the list of all valid partitions (with respect to a given $list_1$), the function will consider each of these partitions (which then determines the bracket structure of $list_2$) and fill up the brackets with all possibilities. Geometrically, this process adds edges between vertices in $S_1(v_0)$ and $S_2(v_0)$, and it is done using the recursive function `generate_special_twoballs`.

A.2. **Function `generate_special_twoballs`.** Given a valid partition, this function fills the brackets of $list_2$ with all possibilities. If we choose the partition 332 in the above example, the first bracket a_5 can be filled with each of the choices $123, 124, \ldots, 234$. If $a_5 = [124]$ is chosen, `avail_outdeg` is updated to $[1, 1, 2, 1]$ before the next bracket a_6 is filled with all possible choices $123, 124, \ldots, 234$. If $a_6 = [134]$ is chosen, `avail_outdeg` is updated to $[0, 1, 1, 0]$ before the next bracket a_7 is filled. This time, the only remaining possibility is $a_7 = [23]$ (since v_1, v_4 are already saturated), finishing the process. Filling of these brackets is done recursively.

A.3. **Function `iso`.** This function checks whether two incomplete 2-balls G, G', represented in standardized form by

$$G = [list_1, list_2, [\ ]], \qquad G' = [list'_1, list'_2, [\ ]]$$

are isomorphic under fixing their centres. We note that G and G' cannot be isomorphic if they have different numbers of vertices or if $list_1 \neq list'_1$. After this preliminary check, we employ all permutations $\sigma : \{1, 2, 3, 4\} \to \{1, 2, 3, 4\}$ that preserve $list_1$, that is

$$\sigma(list_1) := [a_{\sigma(1)\sigma(2)}, \ldots, a_{\sigma(3)\sigma(4)}] = list_1,$$

and apply these permutations to $list_2$, that is

$$\sigma(list_2) := [\sigma(a_5), \ldots, \sigma(a_m)].$$

Here $\sigma(a_j)$ is obtained from the list a_j by replacing each entry i in a_j by $\sigma(i)$. In other words, the permutation of the vertex indices in $S_1(v_0)$ of G induces a corresponding relabeling within $list_2$. We then standardize the new permuted representation $\sigma(list_2)$ by its lexicographic ordering. Then G and G' are isomorphic if and only if one of these modifications of $list_2$ lead to agreement with $list'_2$.

Appendix B. Explicit curvature calculation

In this appendix we briefly explain the theoretical ideas how to calculate curvature. We refer the reader to [CLP17] for more theoretical details and [CKLLS17] for information of the curvature calculator implementation.

The quadratic forms $\Gamma(\cdot,\cdot)(v_0)$ and $\Gamma_2(\cdot,\cdot)(v_0)$ can be represented by matrices $\Gamma(v_0)$ and $\Gamma_2(v_0)$ as follows:

$$\begin{aligned} \Gamma(f,g)(v_0) &= \underline{f}\Gamma(v_0)\underline{g}^T \\ \Gamma_2(f,g)(v_0) &= \underline{f}\Gamma_2(v_0)\underline{g}^T, \end{aligned}$$

where $\underline{f}$ and $\underline{g}$ are the vector representations of f and g. The matrices $\Gamma(v_0)$ and $\Gamma_2(v_0)$ are symmetric with non-zero entries only in $B_1(v_0)$ and $B_2(v_0)$, respectively.

The entries of $\Gamma(v_0)$ and $\Gamma_2(v_0)$ are explicitly given in our case of quartic incomplete 2-balls as follows (see [CLP17, Subsections 2.2 and 2.3]), where the rows and columns are ordered by the vertices $v_0; v_1, \ldots, v_4; v_5, \ldots, v_m$:

$$2\Gamma(v_0) = \left(\begin{array}{c|cccc} 4 & -1 & -1 & -1 & -1 \\ \hline -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{array}\right) \tag{14}$$

and $4\Gamma_2(v_0)$ is given as follows:

$$\left(\begin{array}{c|cccc|cccc} 28 & -7-d^+_{v_1} & -7-d^+_{v_2} & -7-d^+_{v_3} & -7-d^+_{v_4} & d^-_{v_5} & d^-_{v_6} & \cdots & d^-_{v_m} \\ \hline -7-d^+_{v_1} & 13-d^+_{v_1} & 2-4a_{12} & 2-4a_{13} & 2-4a_{14} & -2w_{15} & -2w_{16} & \cdots & -2w_{1m} \\ -7-d^+_{v_2} & 2-4a_{12} & 13-d^+_{v_2} & 2-4a_{23} & 2-4a_{24} & -2w_{25} & -2w_{26} & \cdots & -2w_{2m} \\ -7-d^+_{v_3} & 2-4a_{13} & 2-4a_{23} & 13-d^+_{v_3} & 2-4a_{34} & -2w_{35} & -2w_{36} & \cdots & -2w_{3m} \\ -7-d^+_{v_4} & 2-4a_{14} & 2-4a_{24} & 2-4a_{34} & 13-d^+_{v_4} & -2w_{45} & -2w_{46} & \cdots & -2w_{4m} \\ \hline d^-(v_5) & -2w_{15} & -2w_{25} & -2w_{35} & -2w_{45} & d^-(v_5) & 0 & \cdots & 0 \\ d^-(v_6) & -2w_{16} & -2w_{26} & -2w_{36} & -2w_{46} & 0 & d^-(v_6) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ d^-(v_m) & -2w_{1m} & -2w_{2m} & -2w_{3m} & -2w_{4m} & 0 & 0 & \cdots & d^-(v_m) \end{array}\right) \tag{15}$$

where $w_{ij} = 1$ if $v_i \sim v_j$ and $w_{ij} = 0$ otherwise, and $d^{\pm}_{v_i} := d^{\pm}_{v_0}(v_i)$ to simplify notation. The curvature $\mathcal{K}_\infty(v_0)$ is the solution of the following *semidefinite programming*:

$$\begin{aligned} &\text{maximize } K \\ &\text{subject to } \Gamma_2(v_0) - K\Gamma(v_0) \geq 0. \end{aligned} \tag{16}$$

Note that in the linear combination $\Gamma_2(v_0) - K\Gamma(v_0)$, the smaller matrix $\Gamma(v_0)$ needs to be extended with 0 entries to match the size of $\Gamma_2(v_0)$.

The solution $\mathcal{K}_\infty(v_0) = K$ of (16) is uniquely determined by the following characterization (see [CLP17, Corollary 2.7]):

(1) $\Gamma_2(v_0) - K\Gamma(v_0)$ is positive semidefinite and
(2) $\dim\ker(\Gamma_2(v_0) - K\Gamma(v_0)) \geq 2$.

We finish this appendix with two examples showing how this characterization can be used to verify curvature sharpness of a given incomplete 2-ball.

Example B.1. *We consider the quartic incomplete* 2*-ball with index 2.3 from Table 2, namely*

$$[[1,1,0,0,1,1],[[12],[3],[4]],[]].$$

In this case we obtain $2\Gamma(v_0)$ *as in* (14) *and* $4\Gamma_2(v_0)$ *as in* (15)*:*

$$4\Gamma_2(v_0) = \left(\begin{array}{c|cccc|ccc} 28 & -8 & -8 & -8 & -8 & 2 & 1 & 1 \\ \hline -8 & 12 & -2 & -2 & 2 & -2 & 0 & 0 \\ -8 & -2 & 12 & 2 & -2 & -2 & 0 & 0 \\ -8 & -2 & 2 & 12 & -2 & 0 & -2 & 0 \\ -8 & 2 & -2 & -2 & 12 & 0 & 0 & -2 \\ \hline 2 & -2 & -2 & 0 & 0 & 2 & 0 & 0 \\ 1 & 0 & 0 & -2 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & -2 & 0 & 0 & 1 \end{array}\right).$$

Then $K_\infty(v_0) = 3$ *can be verified by checking that*

$$\Gamma_2(v_0) - 3\Gamma(v_0) = \frac{1}{4}\left(\begin{array}{c|cccc|ccc} 4 & -2 & -2 & -2 & -2 & 2 & 1 & 1 \\ \hline -2 & 6 & -2 & -2 & 2 & -2 & 0 & 0 \\ -2 & -2 & 6 & 2 & -2 & -2 & 0 & 0 \\ -2 & -2 & 2 & 6 & -2 & 0 & -2 & 0 \\ -2 & 2 & -2 & -2 & 6 & 0 & 0 & -2 \\ \hline 2 & -2 & -2 & 0 & 0 & 2 & 0 & 0 \\ 1 & 0 & 0 & -2 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & -2 & 0 & 0 & 1 \end{array}\right).$$

is indeed positive semidefinite and that $\dim\ker(\Gamma_2(v_0) - 3\Gamma(v_0)) = 3$ *with the nullspace spanned by* $(1,1,1,1,1,1,1)^T$, $(-1,\frac{1}{2},-\frac{1}{2},0,0,0,1,1)^T$, *and* $(0,\frac{1}{2},\frac{1}{2},0,0,1,0,0)^T$ *(found via a MAPLE calculation and easily checked by hand). The positive semidefiniteness follows from the fact that the characteristic polynomial of* $4(\Gamma_2(v_0) - 3\Gamma(v_0))$ *is given by*

$$x^8 - 32x^7 + 367x^6 - 1800x^5 + 3360x^4 - 832x^3,$$

and that this polynomial is obviously strictly positive for any value $x < 0$*. This shows that* v_0 *is curvature sharp.*

Example B.2. *We consider the quartic incomplete* 2*-ball given by*

$$[[1,0,0,0,0,1],[[123],[134],[24]],[]].$$

Curvature sharpness at v_0 *requires* $\mathcal{K}_\infty(v_0) = 2.5$ *by criterion* (6). *Thus we have to investigate the matrix*

$$\Gamma_2(v_0) - 2.5\Gamma(v_0) = \frac{1}{4}\left(\begin{array}{c|cccc|ccc} 8 & -4 & -4 & -4 & -4 & 3 & 3 & 2 \\ \hline -4 & 6 & -2 & 2 & 2 & -2 & -2 & 0 \\ -4 & -2 & 6 & 2 & 2 & -2 & 0 & -2 \\ -4 & 2 & 2 & 6 & -2 & -2 & -2 & 0 \\ -4 & 2 & 2 & -2 & 6 & 0 & -2 & -2 \\ \hline 3 & -2 & -2 & -2 & 0 & 3 & 0 & 0 \\ 3 & -2 & 0 & -2 & -2 & 0 & 3 & 0 \\ 2 & 0 & -2 & 0 & -2 & 0 & 0 & 2 \end{array}\right).$$

This matrix is not positive semidefinite since the smallest eigenvalue of this matrix is $-0.148\ldots$ *(found numerically via MAPLE). The non-positive semidefiniteness can also be proved theoretically by using the fact that the characteristic polynomial of* $4(\Gamma_2(v_0) - 2.5\Gamma(v_0))$ *is given by*

$$x^2(x^6 - 40x^5 + 543x^4 - 3032x^3 + 6080x^2 - 1216x - 3584)$$

and that the factor

$$p(x) = x^6 - 40x^5 + 543x^4 - 3032x^3 + 6080x^2 - 1216x - 3584$$

is strictly negative for $x = 0$ *and that* $\lim_{x\to-\infty} p(x) = +\infty$. *The Intermediate Value Theorem tells us that the matrix* $\Gamma_2(v_0) - 2.5\Gamma(v_0)$ *has a negative eigenvalue. Therefore,* v_0 *is not curvature sharp. In fact, a numerical calculation (using MAPLE) shows that* $\mathcal{K}_\infty(v_0) = 2.139\ldots$.

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