

# A classification of graphs through quadratic embedding constants and clique graph insights

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**Abstract:** The quadratic embedding constant (QEC) of a graph  $G$  is a new numeric invariant, which is defined in terms of the distance matrix and is denoted by  $\text{QEC}(G)$ . By observing graph structure of the maximal cliques (clique graph), we show that a graph  $G$  with  $\text{QEC}(G) < -1/2$  admits a “cactus-like” structure. We derive a formula for the quadratic embedding constant of a graph consisting of two maximal cliques. As an application we discuss characterization of graphs along the increasing sequence of  $\text{QEC}(P_d)$ , where  $P_d$  is the path on  $d$  vertices. In particular, we study graphs  $G$  satisfying  $\text{QEC}(G) < \text{QEC}(P_5)$ .

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## 1. Introduction

In the recent paper [22] the *quadratic embedding constant* (*QE constant* for short) of a finite connected graph  $G = (V, E)$  with  $|V| \geq 2$  is defined by

$$\text{QEC}(G) = \max\{\langle f, Df \rangle; f \in C(V), \langle f, f \rangle = 1, \langle 1, f \rangle = 0\}, \quad (1.1)$$

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where  $C(V)$  is the space of all  $\mathbb{R}$ -valued functions on  $V$ ,  $\mathbf{1} \in C(V)$  the constant function taking value 1, and  $\langle \cdot, \cdot \rangle$  the canonical inner product. The QE constant is profoundly related to the quadratic embedding of a graph in a Euclidean space [10, 12, 25, 26] or more generally to Euclidean distance geometry [1, 3, 6, 14]. In fact, it is essential to note that a graph  $G$  admits a quadratic embedding in Euclidean space if and only if  $\text{QEC}(G) \leq 0$ . In recent years, the QE constant has garnered growing interest as a new numeric invariant of graphs. The QE constants of graphs of particular classes are known explicitly, see [5, 11, 17, 19–23], and the formulas in relation to graph operations are established in [16, 18]. Moreover, a table of the QE constants of graphs on  $n \leq 5$  vertices is available [22], where the value of the graph No. 12 on  $n = 5$  vertices is wrong and the correction is found in [4].

With the above mentioned background, we are naturally led to the forward-thinking project of classifying graphs by means of the QE constants. In [4] we initiated an attempt to classify graphs along with  $\text{QEC}(P_d)$ , the QE constant of the path  $P_d$  on  $d \geq 2$  vertices, which forms an increasing sequence as

$$-1 = \text{QEC}(P_2) < \text{QEC}(P_3) < \cdots < \text{QEC}(P_d) < \cdots \rightarrow -\frac{1}{2}. \quad (1.2)$$

In fact, it is known [17] that

$$\text{QEC}(P_d) = -\left(1 + \cos \frac{\pi}{d}\right)^{-1}, \quad d \geq 2. \quad (1.3)$$

In this paper, we study graphs  $G = (V, E)$  with  $\text{QEC}(G) < -1/2$  by means of the *clique graph*  $\Gamma(G)$ . Here the clique graph is a graph  $\Gamma(G) = (\mathcal{V}, \mathcal{E})$ , where  $\mathcal{V}$  is the set of maximal cliques of  $G$  and  $\{H_1, H_2\} \in \mathcal{E}$  if and only if  $H_1 \neq H_2$  and  $H_1 \cap H_2 \neq \emptyset$ . A key result is that the clique graph of a graph  $G$  with  $\text{QEC}(G) < -1/2$  is a tree. Then, combining the result on forbidden subgraphs [4], we conclude that a graph  $G$  with  $\text{QEC}(G) < -1/2$  consists of maximal cliques which form a “cactus-like” structure, for the precise statement see Theorem 1. As an application we discuss graphs  $G$  satisfying  $\text{QEC}(G) < \text{QEC}(P_5)$ .

It is noteworthy that the QE constant provides additional information to the distance spectra and raises interesting questions, for the distance spectra see e.g., [2, 3, 9, 15]. In fact, it is known [16] that  $\delta_2(G) \leq \text{QEC}(G) < \delta_1(G)$ , where  $\delta_1(G)$  and  $\delta_2(G)$  are the largest and the second largest eigenvalues of the distance matrix of  $G$ , respectively. It is straightforward to see that  $\delta_2(G) = \text{QEC}(G)$  holds if the distance matrix of  $G$  has a constant row sum (in some literatures, such a graph is called *transmission regular*). But the converse is not true as the paths  $P_n$  with even  $n$  are counter-examples [17]. In this aspect characterization of graphs satisfying  $\delta_2(G) = \text{QEC}(G)$  is an interesting question. On the other hand, the second largest eigenvalue  $\delta_2(G)$  has been adopted for classifying graphs, in particular, the distance-regular graphs  $G$  with  $\delta_2(G) \leq 0$  are classified [13]. In the recent paper [7] the bicyclic graphs and the split graphs  $G$  with

$\delta_2(G) < -1/2$  are characterized. A detailed comparison is naturally expected to be very interesting and will appear elsewhere.

The paper is organized as follows. In Section 2 we assemble some basic notations for the QE constants. In Section 3 we examine some properties of the clique graph  $\Gamma(G)$  and show a relation between the diameters of  $G$  and  $\Gamma(G)$  (Propositions 5 and 6). In Section 4 we prove the main result (Theorem 1). In Section 5 we determine a graph with exactly two maximal cliques. In Section 6 we discuss graphs  $G$  satisfying  $\text{QEC}(G) < \text{QEC}(P_5)$ . In Appendix we derive a formula for the QE constant of a graph with exactly two maximal cliques.

## 2. Quadratic Embedding Constants

Throughout the paper a graph  $G = (V, E)$  is a pair, where  $V$  is a non-empty finite set and  $E$  is a set of two-element subsets  $\{x, y\} \subset V$ . As usual, elements of  $V$  and  $E$  are respectively called a *vertex* and an *edge*. Two vertices  $x, y \in V$  are called *adjacent* if  $\{x, y\} \in E$ , and we also write  $x \sim y$ . In that case we have  $x \neq y$  necessarily.

For  $s \geq 0$  a sequence of vertices  $x = x_0, x_1, \dots, x_s = y \in V$  is called a *walk* connecting  $x$  and  $y$  of length  $s$  if they are successively adjacent:

$$x = x_0 \sim x_1 \sim \dots \sim x_s = y. \quad (2.1)$$

A graph  $G$  is called *connected* if any pair of vertices are connected by a walk. In this paper a graph is always assumed to be connected unless otherwise stated. The length of a shortest walk connecting two vertices  $x, y \in V$  is called the *graph distance* between  $x$  and  $y$  in  $G$  and is denoted by  $d_G(x, y)$ . A walk in (2.1) is called a *shortest path* connecting  $x$  and  $y$  if  $s = d_G(x, y)$  holds. In that case  $x_0, x_1, \dots, x_s$  are mutually distinct.

As is defined in (1.1), the *QE constant* of a graph  $G = (V, E)$ , denoted by  $\text{QEC}(G)$ , is the conditional maximum of the quadratic function  $\langle f, Df \rangle$  associated to the distance matrix  $D = [d_G(x, y)]$  subject to two constraints  $\langle f, f \rangle = 1$  and  $\langle 1, f \rangle = 0$ .

In this section we assemble some basic results, for more details see e.g., [4, 18, 22]. We first recall a computational formula based on the standard method of Lagrange's multipliers.

**Proposition 1** ([22]). *Let  $D$  be the distance matrix of a graph  $G = (V, E)$  on  $n = |V|$  vertices with  $n \geq 3$ . Let  $\mathcal{S}$  be the set of all stationary points  $(f, \lambda, \mu)$  of*

$$\varphi(f, \lambda, \mu) = \langle f, Df \rangle - \lambda(\langle f, f \rangle - 1) - \mu\langle 1, f \rangle, \quad (2.2)$$

where  $f \in C(V) \cong \mathbb{R}^n$ ,  $\lambda \in \mathbb{R}$  and  $\mu \in \mathbb{R}$ . Then we have

$$\text{QEC}(G) = \max\{\lambda; (f, \lambda, \mu) \in \mathcal{S}\}.$$

In general, a graph  $H = (V', E')$  is called a *subgraph* of  $G = (V, E)$  if  $V' \subset V$  and  $E' \subset E$ . If both  $G$  and  $H$  are connected, they have their own graph distances. If they coincide in such a way that

$$d_H(x, y) = d_G(x, y), \quad x, y \in V',$$

we say that  $H$  is *isometrically embedded* in  $G$ . The next assertions are immediate from definition but useful.

**Proposition 2** ([20, 21]). *Let  $G = (V, E)$  be a graph and  $H = (V', E')$  a subgraph.*

- (1) *If  $H$  is isometrically embedded in  $G$ , then  $H$  is an induced subgraph of  $G$ .*
- (2) *If  $H$  is an induced subgraph of  $G$  and*

$$\text{diam}(H) = \max\{d_H(x, y); x, y \in V'\} \leq 2,$$

*then  $H$  is isometrically embedded in  $G$ .*

**Proposition 3** ([22]). *Let  $G = (V, E)$  and  $H = (V', E')$  be two graphs with  $|V| \geq 2$  and  $|V'| \geq 2$ . If  $H$  is isometrically embedded in  $G$ , we have*

$$\text{QEC}(H) \leq \text{QEC}(G). \tag{2.3}$$

*In particular, (2.3) holds if  $H$  is an induced subgraph of  $G$  and  $\text{diam}(H) \leq 2$ .*

Since any graph  $G = (V, E)$  with  $|V| \geq 2$  contains at least one edge, it has a subgraph  $K_2$  isometrically embedded in  $G$ . It then follows from Proposition 3 that

$$\text{QEC}(G) \geq \text{QEC}(K_2) = -1.$$

Moreover, we have the following assertion, see also Proposition 11.

**Proposition 4** ([4]). *For a graph  $G$  we have  $\text{QEC}(G) = -1$  if and only if  $G$  is a complete graph.*

Thus, in order to determine  $\text{QEC}(G)$  of a graph  $G$  which is not a complete graph, it is sufficient to seek out the stationary points of  $\varphi(f, \lambda, \mu)$  with  $\lambda > -1$  and then to specify the maximum of  $\lambda$  appearing therein.

### 3. Clique Graphs

Most of this section follows a standard argument; however, to avoid ambiguity, we present some basic properties of clique graphs.

Let  $G = (V, E)$  be a graph (always assumed to be finite and connected). For a non-empty subset  $H \subset V$ , the subgraph induced by  $H$  is denoted by  $\langle H \rangle$ . By definition the vertex set of  $\langle H \rangle$  is  $H$  itself and two-element subset  $\{x, y\} \subset H$  belongs to the edge set of  $\langle H \rangle$  if and only if  $\{x, y\} \in E$ . A non-empty subset  $H \subset V$  is called a *clique* of  $G$  if  $\langle H \rangle$  is a complete graph. A clique is called *maximal* if it is maximal in the family of cliques with respect to the inclusion relation. Except for notation, ‘clique’ may also refer to the subgraph it induces.

Obviously, for a clique  $H_0$  there exists a maximal clique  $H$  such that  $H_0 \subset H$ . In particular, for two vertices  $a \sim b$  there exists a maximal clique containing  $\{a, b\}$ .

**Lemma 1.** *Let  $H_1$  and  $H_2$  be maximal cliques of a graph  $G$  such that  $H_1 \neq H_2$ . Then  $H_1 \setminus H_2 \neq \emptyset$  and  $H_2 \setminus H_1 \neq \emptyset$ . Moreover, there exist  $a \in H_1 \setminus H_2$  and  $b \in H_2 \setminus H_1$  such that  $a \not\sim b$ .*

*Proof.* Suppose that  $H_1 \setminus H_2 = \emptyset$  or  $H_2 \setminus H_1 = \emptyset$ . If the former occurs, we have  $H_1 \subset H_2$ . Since both  $H_1$  and  $H_2$  are maximal and  $H_1 \neq H_2$  by assumption, we come to a contradiction.

For the second half of the assertion, suppose that any pair of  $x \in H_1 \setminus H_2$  and  $y \in H_2 \setminus H_1$  are adjacent. We will show that  $H_1 \cup H_2$  is a clique. In fact, take a pair of distinct vertices  $x, y \in H_1 \cup H_2$ . If  $x, y \in H_1$  or  $x, y \in H_2$ , they are adjacent since  $H_1$  and  $H_2$  are cliques. If otherwise, we have  $x \in H_1 \setminus H_2$  and  $y \in H_2 \setminus H_1$  or vice versa, and hence  $x \sim y$  by assumption. Consequently, for any pair of distinct vertices  $x, y \in H_1 \cup H_2$  we have  $x \sim y$ , namely,  $H_1 \cup H_2$  becomes a clique. Since  $H_1 \cup H_2$  contains  $H_1$  and  $H_2$  properly, we come to a contradiction.  $\square$

For a graph  $G = (V, E)$  let  $\mathcal{V}$  be the set of all maximal cliques and  $\mathcal{E}$  the set of two-element subsets  $\{H_1, H_2\} \subset \mathcal{V}$  such that  $H_1 \cap H_2 \neq \emptyset$ . Then  $\Gamma(G) = (\mathcal{V}, \mathcal{E})$  becomes a (in fact, connected) graph, which is called the *clique graph* of  $G$ . Accordingly, for two maximal cliques  $H_1$  and  $H_2$  of  $G$  we write  $H_1 \sim H_2$  if  $H_1 \neq H_2$  and  $H_1 \cap H_2 \neq \emptyset$ . For more information on the clique graph, see e.g., [24, 27].

**Lemma 2.** *The clique graph  $\Gamma(G)$  of a graph  $G$  (always assumed to be connected) is connected.*

*Proof.* Let  $H_1, H_2$  be two maximal cliques such that  $H_1 \neq H_2$ . By Lemma 1 we may choose  $a \in H_1 \setminus H_2$  and  $b \in H_2 \setminus H_1$ . Since  $G$  is connected, there exists a walk connecting  $a$  and  $b$ , say,

$$a = x_0 \sim x_1 \sim \cdots \sim x_s = b,$$

where  $s \geq 1$ . For  $1 \leq i \leq s$  take a maximal clique  $J_i$  containing  $\{x_{i-1}, x_i\}$ . Then  $x_i \in J_i \cap J_{i+1}$  implies that  $J_i = J_{i+1}$  or  $J_i \sim J_{i+1}$ . Moreover, it follows from  $a = x_0 \in H_1 \cap J_1$  that  $H_1 = J_1$  or  $H_1 \sim J_1$ . Similarly,  $H_2 = J_s$  or  $H_2 \sim J_s$ . In any case,  $H_1$  and  $H_2$  are connected by a walk consisting of  $J_1, J_2, \dots, J_s$ .  $\square$

**Example 1.** For a complete graph  $K_n$  with  $n \geq 1$ , a path  $P_n$  with  $n \geq 2$ , and a cycle  $C_n$  with  $n \geq 3$  we have

$$\Gamma(K_n) = K_1, \quad \Gamma(P_n) = P_{n-1}, \quad \Gamma(C_n) = C_n.$$

If every maximal clique of a graph  $G$  is  $K_2$ , the clique graph  $\Gamma(G)$  is nothing else but the line graph of  $G$ . Examples of this type are  $G = P_n$  and  $G = C_n$ .

**Lemma 3.** For  $d \geq 1$  let

$$x_0 \sim x_1 \sim \dots \sim x_d, \tag{3.1}$$

be a shortest path connecting  $x_0$  and  $x_d$ , that is,  $d(x_0, x_d) = d$ . For  $1 \leq i \leq d$  let  $H_i$  be a maximal clique containing  $\{x_{i-1}, x_i\}$ . Then,

$$H_1 \sim H_2 \sim \dots \sim H_d \tag{3.2}$$

and  $d(H_1, H_d) = d - 1$ . Hence (3.2) is a shortest path connecting  $H_1$  and  $H_d$ , and  $H_1, H_2, \dots, H_d$  are mutually distinct.

*Proof.* For  $1 \leq i \leq d - 1$  we have  $x_i \in H_i \cap H_{i+1}$  by definition, and hence  $H_i = H_{i+1}$  or  $H_i \sim H_{i+1}$ . Suppose that  $H_i = H_{i+1}$  occurs. Then  $x_{i-1}, x_i, x_{i+1} \in H_i$  and these three vertices are mutually distinct because (3.1) is a shortest path. Since  $H_i$  is a clique, we have  $x_{i-1} \sim x_{i+1}$ , which contradicts to that (3.1) is a shortest path. Thus we obtain a walk as in (3.2).

We next prove that (3.2) gives rise to a shortest path. Let  $s = d(H_1, H_d)$  and take a shortest path

$$H_1 = J_0 \sim J_1 \sim \dots \sim J_s = H_d.$$

In that case we have

$$s \leq d - 1. \tag{3.3}$$

For  $1 \leq i \leq s$  we take  $y_i \in J_{i-1} \cap J_i$ . Then  $y_1 \sim y_2 \sim \dots \sim y_s$ . Moreover, since  $x_0, y_1 \in H_1 = J_0$  we have  $x_0 = y_1$  or  $x_0 \sim y_1$ . Similarly,  $x_d = y_s$  or  $x_d \sim y_s$ . Thus we obtain a walk connecting  $x_0$  and  $x_d$  whose length is  $s - 1$ ,  $s$  or  $s + 1$ . Hence  $d = d(x_0, x_d) \leq s + 1$ . Combining (3.3) we obtain  $s = d - 1$  and hence  $d(H_1, H_d) = d - 1$  as desired.  $\square$

**Proposition 5.** Let  $G$  be a graph and  $\Gamma(G)$  its clique graph. Then

$$\text{diam}(G) - 1 \leq \text{diam}(\Gamma(G)). \tag{3.4}$$

*Proof.* It is sufficient to show the assertion for a graph  $G$  with  $d = \text{diam}(G) \geq 1$ . We take a shortest path  $x_0 \sim x_1 \sim \cdots \sim x_d$  such that  $d(x_0, x_d) = d$ . Define a sequence of maximal cliques  $H_1, \dots, H_d$  as in Lemma 3. Then we have

$$d - 1 = d(H_1, H_d) \leq \text{diam}(\Gamma(G)),$$

which completes the proof of (3.4).  $\square$

**Lemma 4.** For  $d \geq 1$  let

$$H_0 \sim H_1 \sim \cdots \sim H_d \tag{3.5}$$

be a shortest path connecting  $H_0$  and  $H_d$ , that is  $d(H_0, H_d) = d$ . For  $1 \leq i \leq d$  take a vertex  $x_i \in H_{i-1} \cap H_i$ . Then

$$x_1 \sim x_2 \sim \cdots \sim x_d \tag{3.6}$$

and  $d(x_1, x_d) = d - 1$ . Hence (3.6) is a shortest path connecting  $x_1$  and  $x_d$ , and  $x_1, x_2, \dots, x_d$  are mutually distinct.

*Proof.* For  $1 \leq i \leq d - 1$  we have  $x_i, x_{i+1} \in H_i$  and hence  $x_i = x_{i+1}$  or  $x_i \sim x_{i+1}$ . Suppose that  $x_i = x_{i+1}$  occurs. Then  $x_i = x_{i+1} \in H_{i-1} \cap H_i \cap H_{i+1}$  and hence  $H_{i-1} \cap H_{i+1} \neq \emptyset$ , from which we obtain  $H_{i-1} = H_{i+1}$  or  $H_{i-1} \sim H_{i+1}$ . In any case we come to a contradiction because (3.5) is a shortest path. We have thus obtained a walk as in (3.6).

We next prove that (3.6) gives rise to a shortest path. We set  $s = d(x_1, x_d)$  and take a shortest path connecting  $x_1$  and  $x_d$ , say,

$$x_1 = y_0 \sim y_1 \sim \cdots \sim y_s = x_d.$$

In that case we have

$$s \leq d - 1. \tag{3.7}$$

For  $1 \leq i \leq s$  let  $J_i$  be a maximal clique containing  $\{y_{i-1}, y_i\}$ . It then follows from Lemma 3 that  $d(J_1, J_s) = s - 1$ . Since  $x_1 = y_0 \in H_0 \cap J_1$ , we have  $H_0 = J_1$  or  $H_0 \sim J_1$ . Similarly, we have  $H_d = J_s$  or  $H_d \sim J_s$ . Thus, we obtain a walk connecting  $H_0$  and  $H_d$  of which length is  $s - 1$ ,  $s$  or  $s + 1$ . Hence  $d = d(H_0, H_d) \leq s + 1$ . Combining (3.7), we obtain  $s = d - 1$  and hence  $d(x_1, x_d) = d - 1$  as desired.  $\square$

**Proposition 6.** Let  $G$  be a graph and  $\Gamma(G)$  its clique graph. If  $\Gamma(G)$  is a tree, we have

$$\text{diam}(G) - 1 = \text{diam}(\Gamma(G)). \tag{3.8}$$

*Proof.* Set  $d = \text{diam}(\Gamma(G))$  and take a shortest path

$$H_0 \sim H_1 \sim \cdots \sim H_d, \tag{3.9}$$

where  $d(H_0, H_d) = d$ . For  $1 \leq i \leq d$  take  $x_i \in H_{i-1} \cap H_i$ . By Lemma 4 we have a shortest path  $x_1 \sim x_2 \sim \dots \sim x_d$ . Moreover, we take  $x_0 \in H_0 \setminus H_1$  and  $x_{d+1} \in H_d \setminus H_{d-1}$ . Thus we obtain a walk

$$x_0 \sim x_1 \sim x_2 \sim \dots \sim x_d \sim x_{d+1} \quad (3.10)$$

whose length is  $d + 1$ .

We shall prove that (3.10) is a shortest path. Set  $s = d(x_0, x_{d+1})$  and take a shortest path, say,

$$x_0 = y_0 \sim y_1 \sim y_2 \sim \dots \sim y_s = x_{d+1} \quad (3.11)$$

For  $1 \leq i \leq s$  let  $J_i$  be a maximal clique containing  $\{y_{i-1}, y_i\}$ . By Lemma 3.2 we obtain a shortest path  $J_1 \sim \dots \sim J_s$ , namely,

$$d(J_1, J_s) = s - 1. \quad (3.12)$$

Now note that  $x_0 = y_0 \in H_0 \cap J_1$ . Then we have  $H_0 = J_1$  or  $H_0 \sim J_1$ . Since  $\Gamma(G)$  is a tree, the ends of a diameter (3.9) are pending vertices. Hence  $H_0 \sim J_1$  implies that  $J_1 = H_1$ . In that case we have  $x_0 = y_0 \in H_0 \cap J_1 = H_0 \cap H_1$ . On the other hand, we chose  $x_0 \in H_0 \setminus H_1$ , which is a contradiction. Therefore,  $H_0 \sim J_1$  does not occur and we have  $H_0 = J_1$ . In a similar manner, we see that  $H_d = J_s$ . Consequently, combining (3.12) we come to

$$d = d(H_0, H_d) = d(J_1, J_s) = s - 1.$$

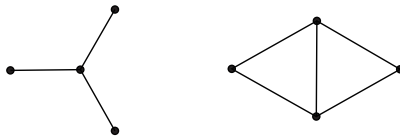
Thus,

$$\text{diam}(\Gamma(G)) = d = s - 1 = d(x_0, x_{d+1}) - 1 \leq \text{diam}(G) - 1.$$

Finally, combining Proposition 5, we obtain the equality (3.8).  $\square$

#### 4. Graphs with $\text{QEC}(G) < -1/2$

The complete bipartite graph  $K_{1,3}$  is called a *claw*. The complete tripartite graph  $K_{1,1,2}$ , which is also obtained by deleting an edge from the complete graph  $K_4$ , is called a *diamond*, see Figure 1. It is essential to note that



**Figure 1.** Claw  $K_{1,3}$  (left) and diamond  $K_{1,1,2}$  (right)



$$\text{QEC}(K_{1,3}) = \text{QEC}(K_{1,1,2}) = -\frac{1}{2}.$$

Since  $\text{diam}(K_{1,3}) = \text{diam}(K_{1,1,2}) = 2$ , we see from Propositions 2 and 3 that if a graph  $G$  contains  $K_{1,3}$  or  $K_{1,1,2}$  as an induced subgraph, we have  $\text{QEC}(G) \geq -1/2$ . Thus, we come to the following criterion.

**Proposition 7 ([4, Corollary 4.1]).** *Any graph  $G$  with  $\text{QEC}(G) < -1/2$  does not contain a claw  $K_{1,3}$  nor a diamond  $K_{1,1,2}$  as an induced subgraph. In short, the claw and diamond are forbidden subgraphs for a graph with  $\text{QEC}(G) < -1/2$ .*

**Lemma 5.** *Let  $G$  be a graph with  $\text{QEC}(G) < -1/2$ . If  $H_1$  and  $H_2$  are maximal cliques of  $G$  with  $H_1 \neq H_2$ , then  $H_1 \cap H_2 = \emptyset$  or  $|H_1 \cap H_2| = 1$ .*

*Proof.* In order to prove the assertion by contradiction, we suppose  $|H_1 \cap H_2| \geq 2$  and take  $x, y \in H_1 \cap H_2$  with  $x \neq y$ . By Lemma 1 there exist  $a \in H_1 \setminus H_2$  and  $b \in H_2 \setminus H_1$  such that  $a \not\sim b$ . Then  $\langle x, y, a, b \rangle$  forms a diamond, which is a forbidden subgraph as stated in Proposition 7.  $\square$

**Lemma 6.** *Let  $G$  be a graph with  $\text{QEC}(G) < -1/2$ . If  $H_1, H_2$  and  $H_3$  are mutually distinct maximal cliques of  $G$ , then  $H_1 \cap H_2 \cap H_3 = \emptyset$ .*

*Proof.* In order to prove the assertion by contradiction we suppose that  $H_1 \cap H_2 \cap H_3 \neq \emptyset$ . Then  $H_1 \cap H_2 \neq \emptyset$  and by Lemma 5 we have  $H_1 \cap H_2 = \{x\}$  for some  $x \in V$ . Hence  $H_2 \cap H_3 = H_3 \cap H_1 = H_1 \cap H_2 \cap H_3 = \{x\}$ . On the other hand, by Lemma 1 there exist  $a \in H_1 \setminus H_2$  and  $b \in H_2 \setminus H_1$  such that  $a \not\sim b$ . Note that there exists  $c \in H_3 \setminus H_1$  such that  $c \not\sim a$ . In fact, if any  $c \in H_3 \setminus H_1$  is adjacent to  $a$ , then  $H_3 \cup \{a\}$  becomes a clique and we come to a contradiction. Thus, we have chosen four vertices  $x, a, b, c$ . There are two cases. In case of  $b \not\sim c$ , the induced subgraph  $\langle x, a, b, c \rangle$  becomes a claw. In case of  $b \sim c$  note that there exist  $c' \in H_3 \setminus H_2$  such that  $c' \not\sim b$ . In fact, if any  $c' \in H_3 \setminus H_2$  is adjacent to  $b$ ,  $H_3 \cup \{b\}$  becomes a clique and we come to a contradiction. Thus, taking  $c' \in H_3 \setminus H_2$  such that  $c' \not\sim b$ , we see that  $\langle x, b, c, c' \rangle$  becomes a diamond. In any case we obtain a forbidden subgraph as stated in Proposition 7 and arrive to a contradiction.  $\square$

**Proposition 8.** *For a graph  $G = (V, E)$  with  $\text{QEC}(G) < -1/2$  the clique graph  $\Gamma(G)$  is a tree.*

*Proof.* Suppose that the clique graph  $\Gamma(G)$  is not a tree and take a smallest cycle, say,

$$H_1 \sim H_2 \sim \cdots \sim H_k \sim H_1, \quad k \geq 3, \quad (4.1)$$

where  $H_i$  is a maximal clique of  $G$  and  $H_i \cap H_{i+1} \neq \emptyset$  for  $1 \leq i \leq k$  (understanding  $H_{k+1} = H_1$ ). It follows from Lemma 5 that there exists a unique vertex  $x_i$  such that  $H_i \cap H_{i+1} = \{x_i\}$  for  $1 \leq i \leq k$ . Then, obviously

$$x_1 \sim x_2 \sim \cdots \sim x_k \sim x_1.$$

(Case 1)  $k = 3$ . In that case  $x_1, x_2, x_3$  are mutually distinct. We note that  $x_1, x_3 \in H_1$  and  $x_2 \notin H_1$ . If  $H_1 = \{x_1, x_3\}$ , namely  $H_1 \setminus \{x_1, x_3\} = \emptyset$ , then  $H_1 \cup \{x_2\}$  becomes a clique containing  $H_1$  properly and we come to a contradiction. Hence  $H_1 \setminus \{x_1, x_3\} \neq \emptyset$ . If any  $y \in H_1 \setminus \{x_1, x_3\}$  is adjacent to  $x_2$ , then  $H_1 \cup \{x_2\}$  becomes a clique containing  $H_1$  properly and we come to a contradiction again. Therefore, there exists  $y \in H_1 \setminus \{x_1, x_3\}$  such that  $y \not\sim x_2$ . Thus,  $\langle x_1, x_2, x_3, y \rangle$  becomes a diamond, which is a forbidden subgraph by Proposition 7. Consequently,  $\Gamma(G)$  does not contain a cycle (4.1) with  $k = 3$ .

(Case 2)  $k \geq 4$ . Using the assumption that (4.1) is a smallest cycle, one can show easily that  $x_1, \dots, x_k$  are mutually distinct.

We first prove that the induced subgraph  $C = \langle x_1, x_2, \dots, x_k \rangle$  becomes a cycle  $C_k$ . In fact, if not, there exist  $1 \leq i, j \leq k$  such that  $i + 1 < j$  and  $x_i \sim x_j$ . Let  $J$  be a maximal clique containing  $\{x_i, x_j\}$ . Then  $x_i \in H_i \cap H_{i+1} \cap J$  and  $x_j \in H_j \cap H_{j+1} \cap J$ . In view of Lemma 6 we obtain  $J = H_i$  or  $J = H_{i+1}$  from the former condition, and similarly  $J = H_j$  or  $J = H_{j+1}$  from the latter. In any case we come to a contradiction against that (4.1) is a smallest cycle.

We next show that the cycle  $C = \langle x_1, x_2, \dots, x_k \rangle \cong C_k$  is isometrically embedded in  $G$ . Suppose otherwise. Then there exist  $1 \leq i, j \leq k$  such that

$$d_G(x_i, x_j) < d_{C_k}(x_i, x_j), \quad (4.2)$$

where the right-hand side is the distance in the cycle  $C_k$ . Without loss of generality, we may assume that  $1 \leq i < j \leq k$ . Then, (4.2) becomes

$$d_G(x_i, x_j) < \min\{j - i, k - (j - i)\}. \quad (4.3)$$

For  $j = i + 1$  we have  $x_i \sim x_j$  and (4.3) does not hold. For  $j = i + 2$  it follows from (4.3) that  $d_G(x_i, x_j) = 1$  and come to a contradiction against the argument in the previous paragraph. Thus, it is sufficient to derive a contradiction from (4.3) for some  $j \geq i + 3$ . Now take a shortest path

$$x_i \sim y_0 \sim y_1 \sim \cdots \sim y_s = x_j, \quad s = d_G(x_i, x_j).$$

For  $1 \leq i \leq s$  take a maximal clique  $J_i$  such that  $\{y_{i-1}, y_i\} \subset J_i$ . Since  $x_i = y_0 \in H_i \cap H_{i+1} \cap J_1$ , by Lemma 6 we have  $J_1 = H_i$  or  $J_1 = H_{i+1}$ . Similarly, we see from  $x_j = y_s \in H_j \cap H_{j+1} \cap J_s$  that  $J_s = H_j$  or  $J_s = H_{j+1}$ . Thus, the path  $J_1 \sim J_2 \sim \cdots \sim J_s$ , which is a shortest path by Lemma 3, gives rise to an alternative

path connecting two vertices of  $C$ , and hence two cyclic walks. We will consider these two cyclic walks in details.

Consider the case where

$$J_1 = H_i, \quad \text{and} \quad J_s = H_j. \quad (4.4)$$

We obtain two cyclic walks:

$$H_1 \sim \cdots \sim H_i = J_1 \sim J_2 \sim \cdots \sim J_s = H_j \sim H_{j+1} \sim \cdots \sim H_k \sim H_1. \quad (4.5)$$

and

$$H_i = J_1 \sim J_2 \sim \cdots \sim J_s = H_j \sim H_{j-1} \sim \cdots \sim H_{i+1} \sim H_i. \quad (4.6)$$

The length of these walks are  $(i-1) + (s-1) + (k-j) + 1 = k + s + i - j$  and  $(s-1) + (j-i) = s + j - i - 1$ , respectively. In view of (4.3) we consider two cases. First, in case of  $s < \min\{j-i, k-(j-i)\} = j-i$  we have  $k + s + i - j < k$ , that is, the length of (4.5) is less than  $k$ . This contradicts to the choice of  $k$ . Second, in case of  $s < \min\{j-i, k-(j-i)\} = k-(j-i)$  we have  $s + j - i - 1 < k - 1$ , that is, the length of (4.5) is less than  $k - 1$ . This contradicts to the choice of  $k$ . Thus (4.4) does not occur.

Other than (4.4) there are three more cases. In each of these cases, in a similar manner as in the previous case, we may find a cycle in  $\Gamma(G)$  which is smaller than (4.1), and come to a contradiction. As a result, the cycle  $C = \langle x_1, x_2, \dots, x_k \rangle \cong C_k$  is isometrically embedded in  $G$ .

We now recall that  $\text{QEC}(C_k) > -1/2$  for any  $k \geq 4$ . In fact, the exact value of  $\text{QEC}(C_k)$  is known [22]. As a consequence of (Case 2), we obtain  $\text{QEC}(G) \geq \text{QEC}(C_k) > -1/2$  and come to a contradiction. Hence,  $\Gamma(G)$  does not contain a smallest cycle (4.1) with  $k \geq 4$ . This completes the proof.  $\square$

Summing up the above results, we state the following

**Theorem 1.** *Let  $G = (V, E)$  be a graph with  $\text{QEC}(G) < -1/2$ . Then the clique graph  $\Gamma(G)$  is a tree. Any pair of adjacent maximal cliques  $H_1$  and  $H_2$  intersect with a single vertex, i.e.,  $|H_1 \cap H_2| = 1$ . Moreover, mutually distinct three maximal cliques  $H_1, H_2$  and  $H_3$  do not intersect, i.e.,  $H_1 \cap H_2 \cap H_3 = \emptyset$ .*

Thus, we say naturally that a graph  $G = (V, E)$  with  $\text{QEC}(G) < -1/2$  is a block graph which admits ‘‘cactus-like’’ structure, see Figure 2. On the other hand, a *cactus* is defined to be a connected graph in which no edge lies on more than one cycle. This definition traces back to [8], though there is ambiguity in the usage in literature. Note that such a cactus is different from our ‘‘cactus-like’’ graph.

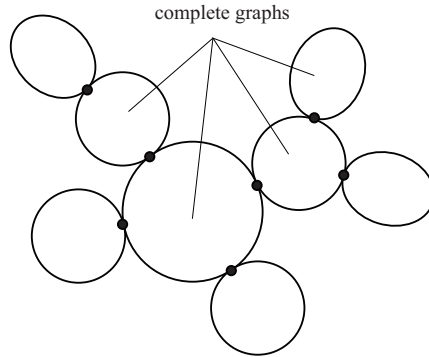


Figure 2. “Cactus-like” graph

## 5. Graphs Consisting of Two Maximal Cliques

For natural numbers  $l \geq 1$ ,  $m > l$  and  $n > l$ , let  $V = \{1, 2, \dots, m+n-l\}$  and consider its two subsets:

$$H_1 = \{1, 2, \dots, m\}, \quad H_2 = \{m-l+1, m-l+2, \dots, m-l+n\}. \quad (5.1)$$

Note that  $V = H_1 \cup H_2$ . Let  $E$  be the set of two-element subsets  $\{x, y\} \subset V$  satisfying  $x, y \in H_1$  or  $x, y \in H_2$ . Then  $G = (V, E)$  becomes a graph which is denoted by  $G = K_m \cup_l K_n$ , see Figure 3. Obviously,  $G = K_m \cup_l K_n$  has exactly two maximal cliques  $H_1$  and  $H_2$ . We will prove that any graph (recall that we always assume that a graph is connected) with exactly two maximal cliques is of this form.

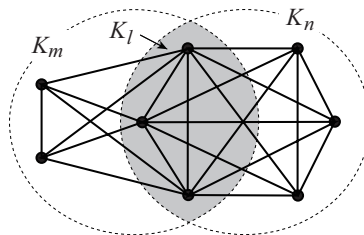


Figure 3. A connected graph consisting of two maximal cliques

**Proposition 9.** *Let  $G = (V, E)$  be a (connected) graph with exactly two maximal cliques. Then there exist three natural numbers  $l \geq 1$ ,  $m > l$  and  $n > l$  such that  $G \cong K_m \cup_l K_n$ .*

Although Proposition 9 pertains to an elementary understanding of graph theory, for later convenience we show an outline of the argument.

**Lemma 7.** *Let  $G = (V, E)$  be a graph with exactly two maximal cliques  $H_1$  and  $H_2$ .*

- (1) *For any  $a \in H_1 \setminus H_2$  and  $b \in H_2 \setminus H_1$  we have  $a \not\sim b$ .*
- (2)  $V = H_1 \cup H_2$ .
- (3)  $H_1 \cap H_2 \neq \emptyset$ .
- (4) *For any  $a \in H_1 \setminus H_2$  and  $b \in H_2 \setminus H_1$  we have  $d_G(a, b) = 2$ .*

*Proof.* (1) Suppose that  $a \in H_1 \setminus H_2$  and  $b \in H_2 \setminus H_1$  are adjacent. There exists a maximal clique containing  $\{a, b\}$ , which is different from  $H_1$  and  $H_2$ . This implies that  $a \not\sim b$  for any pair of  $a \in H_1 \setminus H_2$  and  $b \in H_2 \setminus H_1$ .

(2) In order to prove by contradiction we suppose  $V \neq H_1 \cup H_2$ . Take  $a \in V \setminus (H_1 \cup H_2)$ . Since  $G$  is connected, there exists  $b \in V$  such that  $a \sim b$ . Then a maximal clique containing  $\{a, b\}$  exists and is different from  $H_1$  and from  $H_2$ . We thus come to a contradiction.

(3) Suppose that  $H_1 \cap H_2 = \emptyset$ . Take  $a \in H_1$  and  $b \in H_2$  arbitrarily. Since  $G$  is connected, there exists a walk connecting  $a$  and  $b$ . Since this walk is kept in  $H_1 \cup H_2$  by (2), we may find  $a' \in H_1$  and  $b' \in H_2$  such that  $a' \sim b'$ . This contradicts to the result of (1).

(4) By (1) we know that  $d_G(a, b) \geq 2$ . On the other hand, taking  $x \in H_1 \cap H_2$  we obtain a walk  $a \sim x \sim b$ , which implies that  $d_G(a, b) \leq 2$ .  $\square$

*Proof of Proposition 9.* Let  $H_1$  and  $H_2$  be the two maximal cliques of  $G$ . We set  $m = |H_1|$ ,  $n = |H_2|$  and  $l = |H_1 \cap H_2|$ . By Lemma 7 we see that  $H_1 \cong K_m$ ,  $H_2 \cong K_n$  and  $H_1 \cap H_2 \cong K_l$  with  $l \geq 1$  and  $m, n > l$ . Moreover, there is no edge connecting vertices  $a \in H_1 \setminus H_2$  and  $b \in H_2 \setminus H_1$ . We conclude that  $G \cong K_m \cup_l K_n$ .  $\square$

The distance matrix of  $G = K_m \cup_l K_n$  is easily written down according to (5.1). In fact, taking Lemma 7 (4) into account, we obtain the distance matrix  $D$  in a block-matrix form as follows:

$$D = \begin{bmatrix} J - I & J & J \\ J & J - I & 2J \\ J & 2J & J - I \end{bmatrix}, \quad (5.2)$$

where  $I$  is the identity matrix and  $J$  the matrix whose entries are all one (the sizes of these matrices are understood in the context). Then  $\text{QEC}(G)$  is obtained by means of the basic formula in Proposition 1. The computation is just a routine and is deferred to the Appendix.

**Theorem 2.** *For  $l \geq 1$ ,  $m > l$  and  $n > l$  we have*

$$\text{QEC}(K_m \cup_l K_n) = -1 + \frac{-(m-l)(n-l) + \sqrt{mn(m-l)(n-l)}}{m+n-l}. \quad (5.3)$$

**Corollary 1** ([4, Proposition 4.4]). *Let  $m \geq 2$  and  $n \geq 2$ . Then  $K_m \cup_1 K_n$  is a graph obtained from  $K_m$  and  $K_n$  by concatenating a vertex, in other words, it is the star product  $K_m \cup_1 K_n = K_m * K_n$ , and we have*

$$\begin{aligned} \text{QEC}(K_m \cup_1 K_n) &= \text{QEC}(K_m * K_n) \\ &= \frac{-mn + \sqrt{mn(m-1)(n-1)}}{m+n-1} \\ &= - \left( 1 + \sqrt{\left(1 - \frac{1}{m}\right)\left(1 - \frac{1}{n}\right)} \right)^{-1}. \end{aligned} \quad (5.4)$$

**Corollary 2.** *Let  $m \geq 3$  and  $n \geq 3$ . Then  $K_m \cup_2 K_n$  is a graph obtained from  $K_m$  and  $K_n$  by concatenating an edge and we have*

$$\text{QEC}(K_m \cup_2 K_n) = \frac{-mn + m + n - 2 + \sqrt{mn(m-2)(n-2)}}{m+n-2}. \quad (5.5)$$

**Remark 1.** By changing parameters we obtain an alternative form of (5.3) in Theorem 2. For  $l, m, n \geq 1$  we have

$$\text{QEC}(K_{m+l} \cup_l K_{n+l}) = -1 + \frac{l}{1 + \sqrt{\left(1 + \frac{l}{m}\right)\left(1 + \frac{l}{n}\right)}}.$$

This is useful to discuss estimates of  $\text{QEC}(K_{m+l} \cup_l K_{n+l})$ .

## 6. Characterization of Graphs Along $\text{QEC}(P_d)$

**Proposition 10.** *Let  $d \geq 3$ . If  $\text{QEC}(G) < \text{QEC}(P_d)$ , we have  $\text{diam}(G) \leq d-2$  and  $\text{diam}(\Gamma(G)) \leq d-3$ .*

*Proof.* Suppose that  $\text{diam}(G) > d-2$ . Then  $\text{diam}(G) \geq d-1$  and  $P_d$  is isometrically embedded in  $G$ . By Proposition 3 we obtain  $\text{QEC}(P_d) \leq \text{QEC}(G)$ , which contradicts to the assumption. Therefore, if  $\text{QEC}(G) < \text{QEC}(P_d)$ , we have  $\text{diam}(G) \leq d-2$ . In that case, since  $\text{QEC}(G) < \text{QEC}(P_d) < -1/2$ , it follows from Theorem 1 that  $\Gamma(G)$  is a tree. We then see from Proposition 6 that  $\text{diam}(\Gamma(G)) = \text{diam}(G) - 1 \leq d-3$ .  $\square$

### 6.1. $\text{QEC}(G) < \text{QEC}(P_3)$

For a graph with  $\text{QEC}(G) < \text{QEC}(P_3)$  we have  $\text{diam}(\Gamma(G)) = 0$ , which means that  $G$  has just one maximal clique. Hence  $G = K_n$  with  $n \geq 2$ . Since  $\text{QEC}(K_n) = -1$ , we have the following assertions immediately.

**Proposition 11** ([4]). *For a graph  $G$  we have  $\text{QEC}(G) = \text{QEC}(P_2) = -1$  if and only if  $G = K_n$  with  $n \geq 2$ .*

**Proposition 12** ([4]). *There exists no graph  $G$  such that  $\text{QEC}(P_2) < \text{QEC}(G) < \text{QEC}(P_3) = -2/3$ .*

### 6.2. $\text{QEC}(G) < \text{QEC}(P_4)$

Let  $G$  be a graph satisfying  $\text{QEC}(G) < \text{QEC}(P_4)$ . It follows from Proposition 10 that  $\text{diam}(\Gamma(G)) \leq 1$ , that is,  $\text{diam}(\Gamma(G)) = 0$  or  $\text{diam}(\Gamma(G)) = 1$ . The case of  $\text{diam}(\Gamma(G)) = 0$  is discussed already in Subsection 6.1.

In the case of  $\text{diam}(\Gamma(G)) = 1$ , the clique graph  $\Gamma(G)$  consists of two vertices, which means that  $G$  has exactly two maximal cliques. By Proposition 9 we obtain  $G = K_m \cup_l K_n$  with  $l \geq 1$ ,  $m > l$  and  $n > l$ . On the other hand, since  $\text{QEC}(G) < -1/2$ , we see from Lemma 5 that  $l = 1$ . Thus,  $G$  is necessarily of the form  $G = K_m \cup_1 K_n = K_m * K_n$  with  $m \geq n \geq 2$ .

With the help of the formula in Corollary 1 we may easily determine  $m \geq n \geq 2$  such that  $\text{QEC}(K_m * K_n) < \text{QEC}(P_4) = -(2 - \sqrt{2})$ . As a result we obtain the following assertions.

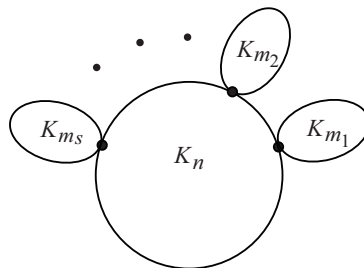
**Proposition 13 ([4]).** *For a graph  $G$  we have  $\text{QEC}(G) = \text{QEC}(P_3) = -2/3$  if and only if  $G = P_3 = K_2 * K_2$ .*

**Proposition 14 ([4]).** *For a graph  $G$  we have  $\text{QEC}(P_3) < \text{QEC}(G) < \text{QEC}(P_4) = -(2 - \sqrt{2})$  if and only if  $G = K_m * K_2$  with  $m \geq 3$  or  $G = K_3 * K_3$ .*

### 6.3. $\text{QEC}(G) < \text{QEC}(P_5)$

If a graph  $G$  satisfies  $\text{QEC}(G) < \text{QEC}(P_5) = -(5 - \sqrt{5})/5$ , then  $\text{diam}(\Gamma(G)) \leq 2$ . The case of  $\text{diam}(\Gamma(G)) = 0$  is already discussed in Subsection 6.1. If  $\text{diam}(\Gamma(G)) = 1$ , we have  $G = K_m * K_n$  with  $m \geq n \geq 2$ . Then, as is discussed in Subsection 6.2, we may employ the explicit formula for  $\text{QEC}(K_m * K_n)$  in Corollary 1. The result will be stated in Propositions 15 and 16.

Consider the case of  $\text{diam}(\Gamma(G)) = 2$ . Since  $\Gamma(G)$  is a tree, it is necessarily a star  $\Gamma(G) = K_{1,s}$  with  $s \geq 2$ . Then  $G$  is a graph obtained as follows: Let  $n \geq s$  and  $m_1 \geq m_2 \geq \dots \geq m_s \geq 2$ . We choose  $s$  vertices from  $K_n$  and to each of the  $s$  vertices we make a star product with  $K_{m_1}, \dots, K_{m_s}$ , see Figure 4. Such a graph is denoted by  $G = K_n * (K_{m_1}, \dots, K_{m_s})$ .



**Figure 4.**  $K_n * (K_{m_1}, \dots, K_{m_s})$

**Lemma 8.** Consider two graphs  $G = K_n * (K_{m_1}, \dots, K_{m_s})$  with  $n \geq s$ ,  $m_1 \geq m_2 \geq \dots \geq m_s \geq 2$ , and  $G' = K_{n'} * (K_{m'_1}, \dots, K_{m'_r})$  with  $n' \geq r$  and  $m'_1 \geq m'_2 \geq \dots \geq m'_r \geq 2$ . If  $n' \leq n$ ,  $r \leq s$ ,  $m'_1 \leq m_1, \dots, m'_r \leq m_r$ , then  $G'$  is isometrically embedded in  $G$ . Hence  $\text{QEC}(G') \leq \text{QEC}(G)$ .

*Proof.* Obvious. □

**Lemma 9.** Let  $n \geq s \geq 2$  and  $m_1 \geq m_2 \geq \dots \geq m_s \geq 2$ . If  $m_1 \geq 3$ , we have

$$\text{QEC}(P_4) < \text{QEC}(K_n * (K_{m_1}, \dots, K_{m_s})).$$

*Proof.* It is known that

$$\text{QEC}(K_2 * (K_3, K_2)) = -\frac{2(6 - \sqrt{21})}{5} \approx -0.5669,$$

see [22], where  $K_2 * (K_3, K_2)$  is referred to as No.5-7. Then we have

$$\text{QEC}(P_4) < \text{QEC}(K_2 * (K_3, K_2)) < \text{QEC}(P_5).$$

On the other hand, for  $n \geq s \geq 2$  and  $m_1 \geq 3$ ,  $K_n * (K_{m_1}, \dots, K_{m_s})$  contains  $K_2 * (K_3, K_2)$  as an isometrically embedded subgraph. Hence

$$\text{QEC}(P_4) < \text{QEC}(K_2 * (K_3, K_2)) \leq \text{QEC}(K_n * (K_{m_1}, \dots, K_{m_s})),$$

as desired. □

**Lemma 10** ([4, Theorem 4.3]). For  $n \geq s \geq 2$  we have

$$\text{QEC}(K_n * \overbrace{(K_2, \dots, K_2)}^{s \text{ times}}) = -(2 - \sqrt{2}) = \text{QEC}(P_4).$$

**Proposition 15.** For a graph  $G$  we have  $\text{QEC}(G) = \text{QEC}(P_4) = -(2 - \sqrt{2})$  if and only if  $G = K_4 * K_3$  or  $G = K_n * (K_2, \dots, K_2)$  ( $K_2$  appears  $s$  times) with  $n \geq s \geq 2$ .

*Proof.* As is discussed in Subsection 6.2, a graph  $G$  with  $\text{diam}(\Gamma(G)) = 1$  is of the form  $K_m * K_n$  with  $m \geq n \geq 2$ . Then, using the explicit formula for  $\text{QEC}(K_m * K_n)$  in Corollary 1, we see easily that  $\text{QEC}(K_m * K_n) = \text{QEC}(P_4)$  if and only if  $m = 4$  and  $n = 3$ .

A graph  $G$  with  $\text{diam}(\Gamma(G)) = 2$  is of the form  $G = K_n * (K_{m_1}, \dots, K_{m_s})$  with  $n \geq s \geq 2$  and  $m_1 \geq m_2 \geq \dots \geq m_s \geq 2$ . By Lemma 9,  $\text{QEC}(G) \leq \text{QEC}(P_4)$  may occur only when  $m_1 = m_2 = \dots = m_s = 2$ . On the other hand, in that case, the equality  $\text{QEC}(G) = \text{QEC}(P_4)$  holds by Lemma 10. □



**Proposition 16.** For  $m \geq n \geq 2$  we have  $\text{QEC}(P_4) < \text{QEC}(K_m * K_n) < \text{QEC}(P_5)$  if and only if

- (i)  $n = 3$  and  $5 \leq m \leq 54$ ;
- (ii)  $n = 4$  and  $4 \leq m \leq 7$ ;
- (iii)  $n = m = 5$ .

*Proof.* Straightforward by the explicit formula for  $\text{QEC}(K_m * K_n)$ .  $\square$

By Proposition 16 all graphs  $G$  such that  $\text{QEC}(P_4) < \text{QEC}(G) < \text{QEC}(P_5)$  with  $\text{diam}(\Gamma(G)) = 1$  are determined. The case of  $\text{diam}(\Gamma(G)) = 2$ , i.e.,  $G = K_n * (K_{m_1}, \dots, K_{m_s})$  remains to be checked. The work in this line is in progress.

### Appendix: Calculating $\text{QEC}(K_m \cup_l K_n)$

Let  $D$  be the distance matrix of  $G = K_m \cup_l K_n$ , where  $l \geq 1$  and  $m, n > l$ . Using the block-matrix form of  $D$  as in (5.2), we will calculate  $\text{QEC}(G)$  explicitly.

For  $f \in \mathbb{R}^l$ ,  $g \in \mathbb{R}^{m-l}$  and  $h \in \mathbb{R}^{n-l}$  we set

$$\begin{aligned} \psi(f, g, h) &= \left\langle \begin{bmatrix} f \\ g \\ h \end{bmatrix}, D \begin{bmatrix} f \\ g \\ h \end{bmatrix} \right\rangle \\ &= \langle 1, f \rangle^2 + \langle 1, g \rangle^2 + \langle 1, h \rangle^2 - \langle f, f \rangle^2 - \langle g, g \rangle^2 - \langle h, h \rangle^2 \\ &\quad + 2\langle 1, f \rangle \langle 1, g \rangle + 2\langle 1, f \rangle \langle 1, h \rangle + 4\langle 1, g \rangle \langle 1, h \rangle \end{aligned}$$

and

$$\begin{aligned} \varphi(f, g, h, \lambda, \mu) &= \psi(f, g, h) - \lambda(\langle f, f \rangle + \langle g, g \rangle + \langle h, h \rangle - 1) \\ &\quad - \mu(\langle 1, f \rangle + \langle 1, g \rangle + \langle 1, h \rangle). \end{aligned} \tag{A.1}$$

It then follows from Proposition 1 that  $\text{QEC}(G)$  coincides with the maximum of  $\lambda \in \mathbb{R}$  appearing in the stationary points of  $\psi(f, g, h, \lambda, \mu)$ . Since  $G$  is not complete, it is sufficient to explore stationary points of  $\psi(f, g, h, \lambda, \mu)$  with  $\lambda > -1$ .

By direct computation together with condition

$$\langle 1, f \rangle + \langle 1, g \rangle + \langle 1, h \rangle = 0$$

we have

$$\frac{\partial \varphi}{\partial f_i} = -2(\lambda + 1)f_i - \mu = 0. \tag{A.2}$$

Then we see that  $f_i$  is constant independent of  $1 \leq i \leq l$ , say  $f_i = \xi$ . Thus, (A.2) becomes

$$\xi = -\frac{1}{\lambda+1} \cdot \frac{\mu}{2}. \quad (\text{A.3})$$

(From the beginning we may assume that  $\lambda > -1$  as noted before.) Similarly, it follows from  $\partial\varphi/\partial g_i = \partial\varphi/\partial h_i = 0$  that  $g_i$  and  $h_i$  are respectively constant. Setting  $g_i = \eta$  and  $h_i = \zeta$ , we obtain

$$(\lambda+1)\eta - (n-l)\zeta = -\frac{\mu}{2}, \quad (\text{A.4})$$

$$-(m-l)\eta + (\lambda+1)\zeta = -\frac{\mu}{2}, \quad (\text{A.5})$$

and the constraints become

$$l\xi + (m-l)\eta + (n-l)\zeta = 0, \quad (\text{A.6})$$

$$l\xi^2 + (m-l)\eta^2 + (n-l)\zeta^2 = 1. \quad (\text{A.7})$$

Our task is to solve the system of equations (A.3)–(A.7).

In view of (A.4) and (A.5) we set

$$\Delta = \det \begin{bmatrix} \lambda+1 & -(n-l) \\ -(m-l) & \lambda+1 \end{bmatrix} = (\lambda+1)^2 - (m-l)(n-l). \quad (\text{A.8})$$

(Case I)  $\Delta \neq 0$ . The equations (A.4) and (A.5) have a unique solution:

$$\eta = -\frac{\lambda+n+1-l}{\Delta} \cdot \frac{\mu}{2}, \quad \zeta = -\frac{\lambda+m+1-l}{\Delta} \cdot \frac{\mu}{2}. \quad (\text{A.9})$$

Inserting (A.3) and (A.9) into (A.6), we obtain

$$l\Delta + (\lambda+1)\{(m-l)(\lambda+n+1-l) + (n-l)(\lambda+m+1-l)\} = 0 \quad (\text{A.10})$$

after simple calculation. The solutions are easily written down as

$$\lambda_{\pm} = -1 + \frac{-(m-l)(n-l) \pm \sqrt{mn(m-l)(n-l)}}{m+n-l}.$$

Checking that  $\lambda_+ \neq -1$  and  $\Delta \neq 0$  for  $\lambda = \lambda_+$ , we see that  $\lambda_+$  is a candidate of  $\text{QEC}(G)$ .

(Case II)  $\Delta = 0$ . From (A.4) and (A.5) we obtain

$$(\lambda+n-l+1)\frac{\mu}{2} = 0, \quad (\lambda+m-l+1)\frac{\mu}{2} = 0.$$

If  $m \neq n$ , we obtain  $\mu = 0$  and  $\xi = \eta = \zeta = 0$ , which do not fulfill (A.7). Hence there is no stationary points. Assume that  $m = n$ . Then  $\lambda = -1 - (m - l)$  appears in the stationary points. However, since we are only interested in  $\lambda > -1$ , there exists no candidate for our  $\text{QEC}(G)$  in the case of  $\Delta = 0$ .

Finally, we conclude from (Case I) and (Case II) that  $\lambda_+ = \text{QEC}(G)$ .

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**Data Availability.** Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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