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Determining finite connected graphs along the quadratic embedding constants of paths

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Abstract

The QE constant of a finite connected graph G, denoted by $\mathrm{QEC}(G)$, is by definition the maximum of the quadratic function associated to the distance matrix on a certain sphere of codimension two. We prove that the QE constants of paths P_n form a strictly increasing sequence converging to $-1/2$. Then we formulate the problem of determining all the graphs G satisfying $\mathrm{QEC}(P_n) \le \mathrm{QEC}(G) < \mathrm{QEC}(P_{n+1})$. The answer is given for $n = 2$ and $n = 3$ by exploiting forbidden subgraphs for $\mathrm{QEC}(G) < -1/2$ and the explicit QE constants of star products of the complete graphs.

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1. Introduction

Let $G = (V, E)$ be a finite connected graph with $|V| = n \ge 2$ and $D = [d(i, j)]_{i,j\in V}$ the distance matrix of G. The *quadratic embedding constant* (*QE constant* for short) of G is defined by

$$\mathrm{QEC}(G) = \max\{\langle f, Df\rangle \,;\, f \in C(V),\, \langle f, f\rangle = 1,\, \langle \mathbf{1}, f\rangle = 0\}, \tag{1}$$

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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 was first introduced for the quantitative study of quadratic embedding of graphs in Euclidean spaces [17, 18]. In particular, a graph G admits a quadratic embedding (in this case we say that G is *of QE class*) if and only if $\mathrm{QEC}(G) \le 0$. Thus, our study is closely related to the so-called Euclidean distance geometry [6, 10, 11, 13]. Moreover, it is noteworthy that $\mathrm{QEC}(G) \le 0$ is equivalent to the positive definiteness of the Q-matrix $Q = [q^{d(i,j)}]$ for all $0 \le q \le 1$. This property, first proved by Haagerup [8] for trees and later by Bożejko [5] for general star products, has many applications in harmonic analysis and quantum probability, see [4, 15, 16] and references cited therein.

It is also interesting to observe a close relation between the QE constants and the distance spectra. In fact, for a finite connected graph we have

$$\lambda_2(G) \le \mathrm{QEC}(G) < \lambda_1(G),$$

where $\lambda_1(G)$ and $\lambda_2(G)$ are respectively the largest and the second largest eigenvalues of the distance matrix of G. It is straightforward to see that $\lambda_2(G) = \mathrm{QEC}(G)$ 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 provide counter-examples. In this aspect characterization of graphs satisfying $\lambda_2(G) = \mathrm{QEC}(G)$ is an interesting problem. In fact, the second largest eigenvalue $\lambda_2(G)$ has been adopted for classifying graphs see e.g., [12]. For generalities of distance spectra see also [1, 2, 3, 9].

In this paper, we initiate the project of characterizing finite connected grahs in terms of the QE constants. Our idea is based on the fact that the QE constants of paths form a strictly increasing sequence:

$$\mathrm{QEC}(P_2) < \mathrm{QEC}(P_3) < \cdots < \mathrm{QEC}(P_n) < \mathrm{QEC}(P_{n+1}) < \cdots \to -\frac{1}{2}\,. \tag{2}$$

Then a natural question arises to determine finite connected graphs along the above QE constants. More precisely, we are interested in the family of graphs G satisfying

$$\mathrm{QEC}(P_n) \le \mathrm{QEC}(G) < \mathrm{QEC}(P_{n+1}), \qquad n \ge 2. \tag{3}$$

The main goal of this paper is to give the answer to the first two cases of $n = 2, 3$.

This paper is organized as follows: In Section 2 we give a quick review on the QE constant, for more details see [14, 18].

In Section 3 we derive a general criterion for the strict inequality

$$\mathrm{QEC}(G) < \mathrm{QEC}(G \star K_{m+1}),$$

where $G \star K_{m+1}$ is the star product, namely, the graph obtained by joining a graph G and the complete graph K_{m+1} at a single vertex, see Theorem 3.1. We then prove that the QE constants of paths form a strictly increasing sequence as in (2), see Theorem 3.2.

In Section 4 we prove the main results. Case of $n = 2$ is simple, in fact, condition (3) characterizes the complete graphs, see Theorem 4.1. For a general case the first useful result is that any graph with $\mathrm{QEC}(G) < -1/2$ is diamond-free, claw-free, C_4-free and C_5-free, see Corollary 4.1. Then, using the explicit values of $\mathrm{QEC}(K_m \star K_n)$ we obtain an explicit list for case of $n = 3$, that is, a series of graphs $K_n \star K_2$ with $n \geq 2$ and one sporadic $K_3 \star K_3$, see Theorem 4.2. As a result, $\mathrm{QEC}(P_4)$ is the smallest accumulation point of the QE constants. We also provide examples of graphs G satisfying $\mathrm{QEC}(G) = \mathrm{QEC}(P_4)$.

2. Quadratic Embedding Constants

2.1. Definition and Basic Properties

A graph $G = (V, E)$ is a pair of a non-empty set V of vertices and a set E of edges, i.e., E is a subset of $\{\{i, j\}\,;\, i, j \in V, i \neq j\}$. A graph is called finite if V is a finite set. Throughout this paper by a graph we mean a finite graph.

If $\{i, j\} \in E$, we write $i \sim j$ for simplicity. A finite sequence of vertices $i_0, i_1, \dots, i_m \in V$ is called an m*-step walk* if $i_0 \sim i_1 \sim \cdots \sim i_m$. In that case we say that i_0 and i_m are connected by a walk of length m. A graph is called *connected* if any pair of vertices are connected by a walk.

Let $G = (V, E)$ be a connected graph. For $i, j \in V$ with $i \neq j$ let $d(i, j) = d_G(i, j)$ denote the length of a shortest walk connecting i and j. By definition we set $d(i, i) = 0$. Then $d(i, j)$ becomes a metric on V, which we call the *graph distance*. The *diameter* of G is defined by

$$\mathrm{diam}(G) = \max\{d(i, j)\,;\, i, j \in V\}.$$

The *distance matrix* of G is defined by

$$D = D_G = [d(i, j)]_{i,j \in V}\,.$$

Let $G = (V, E)$ be a connected graph with $|V| \geq 2$. The *quadratic embedding constant* (*QE constant* for short) of G is defined by

$$\mathrm{QEC}(G) = \max\{\langle f, Df\rangle\,;\, f \in C(V),\, \langle f, f\rangle = 1,\, \langle \mathbf{1}, f\rangle = 0\}, \tag{4}$$

where $C(V)$ is the space of all $\mathbb{R}$-valued functions on V and $\langle \cdot, \cdot \rangle$ the canonical inner product on $C(V)$. Furthermore, $\mathbf{1}$ is the constant function defined by $\mathbf{1}(x) = 1$ for all $x \in V$, and $\langle \mathbf{1}, f\rangle = \sum_{x \in V} f(x)$. Indeed, identifying $C(V)$ with $\mathbb{R}^n$, $n = |V|$, we see that the domain

$$\{f \in C(V)\,;\, \langle f, f\rangle = 1,\, \langle \mathbf{1}, f\rangle = 0\}$$

is a compact manifold (in fact, a sphere of $n-2$ dimension). Hence the quadratic function $\langle f, Df\rangle$ attains the maximum on the above domain.

Proposition 2.1. *Let $G = (V, E)$ be a connected graph with $|V| \geq 2$, and $D = [d(i, j)]$ the distance matrix. Then the following conditions are equivalent:*

(i) *G is of QE class, that is, there exist a Euclidean space $\mathcal{H}$ and a map $\varphi : V \to \mathcal{H}$ such that*

$$\|\varphi(i) - \varphi(j)\|^2 = d(i, j), \qquad i, j \in V.$$

(ii) *D is conditionally negative definite, that is,*

$$\langle f, Df \rangle \le 0 \quad \textit{for all } f \in C(V) \textit{ with } \langle \mathbf{1}, f \rangle = 0.$$

(iii) $\mathrm{QEC}(G) \le 0$.

The map $\varphi : V \to \mathcal{H}$ in the above condition (i) is called a *quadratic embedding* of G. The above result is essentially due to Schoenberg [19, 20] and motivated us to introduce the QE constant.

The graphs of QE class include the complete graphs K_n ($n \ge 2$), paths P_n ($n \ge 2$), and cycles C_n ($n \ge 3$). In fact,

$$\mathrm{QEC}(K_n) = -1, \qquad n \ge 2, \tag{5}$$

and

$$\mathrm{QEC}(C_{2n+1}) = -\frac{1}{4\cos^2 \dfrac{\pi}{2n+1}}, \qquad \mathrm{QEC}(C_{2n+2}) = 0, \qquad n \ge 1, \tag{6}$$

while a closed expression for $\mathrm{QEC}(P_n)$ is not known. It is also noted that the QE constant of a tree is negative. In fact, for any tree G on n vertices we have

$$\mathrm{QEC}(G) \le -\frac{2}{2n-3}, \qquad n \ge 3. \tag{7}$$

However, (7) is a rather rough estimate and its refinement is an interesting question, see [14, Section 5].

Proposition 2.2. *Let $G = (V, E)$ be a connected graph and $H = (W, F)$ a connected subgraph of G with $|W| \ge 2$. If H is isometrically embedded in G, i.e.,*

$$d_H(i, j) = d_G(i, j) \quad \textit{for all } i, j \in W,$$

then we have

$$\mathrm{QEC}(H) \le \mathrm{QEC}(G).$$

Proof. Take $f \in C(W)$ such that

$$\mathrm{QEC}(H) = \langle f, D_H f \rangle, \quad \langle f, f \rangle_W = 1, \quad \langle \mathbf{1}, f \rangle_W = 0,$$

where $\langle \cdot, \cdot \rangle_W$ denotes the inner product on $C(W)$. Define $\tilde{f} \in C(V)$ in such a way that $\tilde{f}(x) = f(x)$ for $x \in W$ and $\tilde{f}(x) = 0$ otherwise. Then $\tilde{f}$ satisfies $\langle \tilde{f}, \tilde{f} \rangle_V = 1$ and $\langle \mathbf{1}, \tilde{f} \rangle_V = 0$. Since H is isometrically embedded in G, the distance matrix D_H is a submatrix of D_G. Hence,

$$\mathrm{QEC}(H) = \langle f, D_H f \rangle = \langle \tilde{f}, D_G \tilde{f} \rangle,$$

where the last quantity is bounded by $\mathrm{QEC}(G)$ by definition. □

Corollary 2.1. *Let P_n be the path on n vertices. Then we have*

$$\mathrm{QEC}(P_2) \le \mathrm{QEC}(P_3) \le \cdots \le \mathrm{QEC}(P_n) \le \mathrm{QEC}(P_{n+1}) \le \cdots. \tag{8}$$

Corollary 2.2. *Let $G = (V, E)$ be a connected graph with $|V| \ge 2$.*

(1) *If* $\mathrm{diam}(G) \ge d$*, then* $\mathrm{QEC}(P_{d+1}) \le \mathrm{QEC}(G)$.
(2) *If* $\mathrm{QEC}(G) < \mathrm{QEC}(P_{d+1})$*, then* $\mathrm{diam}(G) \le d - 1$.

The proofs are straightforward from Proposition 2.2. In fact, as is shown in Subsection 3.2, the inequalities in (8) are strict.

Next we derive a useful criterion for isometric embedding.

Lemma 2.1. *Let $G = (V, E)$ be a connected graph and $H = (W, F)$ a connected subgraph.*

(1) *If H is isometrically embedded, then H is an induced subgraph of G.*
(2) *If H is an induced subgraph of G and* $\mathrm{diam}\,(H) \le 2$*, then H is isometrically embedded in G.*

Proof. Let d_G and d_H be the graph distances of G and H, respectively.

(1) Let $i, j \in W$ and assume that they are adjacent in G. Then $d_G(i, j) = 1$ and by assumption we have $d_H(i, j) = 1$, which means that i and j are adjacent in H too. Therefore, H is an induced subgraph of G.

(2) Let $i, j \in W$. Then $d_H(i, j) \le 2$ by assumption. If $d_H(i, j) = 0$, then $i = j$ and hence $d_G(i, j) = 0$. Suppose that $d_H(i, j) = 1$. Then i and j are adjacent in H, so are in G. Hence $d_G(i, j) = 1$. Finally, suppose that $d_H(i, j) = 2$. Obviously, $i \ne j$ so that $1 \le d_G(i, j) \le 2$. If $d_G(i, j) = 1$, then i and j are adjacent in G and so are in H since H is an induced subgraph. Then we obtain $d_H(i, j) = 1$, which is contradiction. Therefore, we have $d_G(i, j) = 2$. Consequently, $d_H(i, j) = d_G(i, j)$ for all $i, j \in W$, which means that H is isometrically embedded in G. □

Proposition 2.3. *Let G be a connected graph, and H a connected and induced subgraph of G. If* $\mathrm{diam}(H) \le 2$*, we have*

$$\mathrm{QEC}(H) \le \mathrm{QEC}(G).$$

Proof. It follows from Lemma 2.1 (2) that H is isometrically embedded in G. Then, by Proposition 2.2 we see that $\mathrm{QEC}(H) \le \mathrm{QEC}(G)$. □

2.2. Calculating QE Constants

Let G be a connected graph on $V = \{1, 2, \ldots, n\}$ and identify $C(V)$ with $\mathbb{R}^n$ in a natural manner. Recall that $\mathrm{QEC}(G)$ is the conditional maximum of the quadratic function $\langle f, Df \rangle$, $f = [f_i] = [f(i)] \in C(V) \cong \mathbb{R}^n$, subject to

$$\langle f, f \rangle = \sum_{i=1}^{n} f_i^2 = 1, \tag{9}$$

$$\langle \mathbf{1}, f \rangle = \sum_{i=1}^{n} f_i = 0. \tag{10}$$

The method of Lagrange multipliers is applied to calculating QE constants. For later use we review it quickly, for more details see [18].

First we set

$$F(f,\lambda,\mu)=\langle f,Df\rangle-\lambda(\langle f,f\rangle-1)-\mu\langle\mathbf{1},f\rangle, \tag{11}$$

where $f=[f_i]\in\mathbb{R}^n$, $\lambda\in\mathbb{R}$ and $\mu\in\mathbb{R}$. Since conditions (9) and (10) define a sphere of $n-2$ dimension, which is smooth and compact, the conditional maximum of $\langle f,Df\rangle$ under question is attained at a stationary points of $F(f,\lambda,\mu)$.

Let $\mathcal{S}$ be the set of stationary points of $F(f,\lambda,\mu)$, that is,

$$\mathcal{S}=\left\{(f=[f_i],\lambda,\mu)\in\mathbb{R}^n\times\mathbb{R}\times\mathbb{R}\,,\;\frac{\partial F}{\partial f_i}=\frac{\partial F}{\partial\lambda}=\frac{\partial F}{\partial\mu}=0\right\}.$$

Taking the derivatives of (11), we obtain

$$\frac{\partial F}{\partial f_i}=2\langle e_i,Df\rangle-2\lambda\langle e_i,f\rangle-\mu\langle\mathbf{1},e_i\rangle=\langle e_i,2(D-\lambda)f-\mu\mathbf{1}\rangle,$$

where $\{e_i\}$ is the canonical basis of $\mathbb{R}^n$. Hence $\partial F/\partial f_i=0$ for all $1\le i\le n$ if and only if $2(D-\lambda)f-\mu\mathbf{1}=0$, that is,

$$(D-\lambda)f=\frac{\mu}{2}\,\mathbf{1}. \tag{12}$$

Thus, $\mathcal{S}$ is the set of $(f,\lambda,\mu)\in\mathbb{R}^n\times\mathbb{R}\times\mathbb{R}$ satisfying (9), (10) and (12). On the other hand, for $(f,\lambda,\mu)\in\mathcal{S}$ we have

$$\langle f,Df\rangle=\left\langle f,\lambda f+\frac{\mu}{2}\,\mathbf{1}\right\rangle=\lambda\langle f,f\rangle+\frac{\mu}{2}\langle f,\mathbf{1}\rangle=\lambda. \tag{13}$$

Thus we come to the following useful result.

Proposition 2.4. *Let G be a connected graph on $n\ge 3$ vertices and $\mathcal{S}$ the set of stationary points of $F(f,\lambda,\mu)$ defined by* (11)*. Then we have*

$$\mathrm{QEC}(G)=\max\{\lambda\in\mathbb{R}\,;\,(f,\lambda,\mu)\in\mathcal{S}\text{ for some } f\in\mathbb{R}^n \text{ and } \mu\in\mathbb{R}\}.$$

3. QE Constants of Paths

3.1. A Criterion for $\mathrm{QEC}(G)<\mathrm{QEC}(G\star K_{m+1})$

Let G_1 and G_2 be two graphs with disjoint vertex sets. Choose o_1 and o_2 as distinguished vertices of G_1 and G_2, respectively. A *star product* of G_1 and G_2 with respect to o_1 and o_2 is (informally) defined to be the graph obtained by joining G_1 and G_2 at the distinguished vertices o_1 and o_2. If there is no danger of confusion, the star product is denoted simply by $G_1\star G_2$.

In this subsection we consider the case where G_1 is an arbitrary connected graph and G_2 a complete graph. To be precise, for $n\ge 2$ and $m\ge 1$ let $G=(V,E)$ be a connected graph on $V=\{1,2,\dots,n\}$ and K_{m+1} the complete graph on $\{n,n+1,\dots,n+m\}$. We set

$$\tilde{V}=V\cup\{n,n+1,\dots,n+m\}=\{1,2,\dots,n+m\},$$

and

$$\tilde{E}=E\cup\{\{i,j\}\,;\,n\le i<j\le n+m\}.$$

Then $\tilde{G} = (\tilde{V}, \tilde{E})$ becomes the star product of G and K_{m+1}, which we denote simply by $\tilde{G} = G \star K_{m+1}$. Since G is isometrically embedded in $\tilde{G}$, it follows from Proposition 2.2 that

$$\mathrm{QEC}(G) \le \mathrm{QEC}(\tilde{G}) = \mathrm{QEC}(G \star K_{m+1}). \tag{14}$$

We are interested in when the inequality (14) becomes strict.

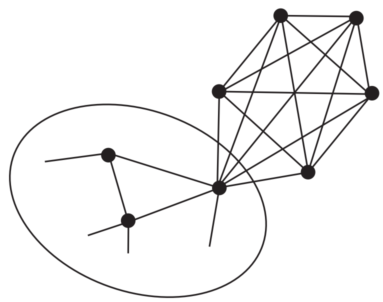

Figure 1. $G \star K_{m+1}$ ($m = 5$).

Let $D = D_G = [d(i,j)]$ and $\tilde{D} = D_{\tilde{G}}$ be the distance matrices of G and $\tilde{G}$, respectively. Then we have

$$\tilde{D} = \left[\begin{array}{c|c} D & S \\ \hline S^T & J - I \end{array}\right], \tag{15}$$

where $S = [s(i,j)]$ is the $n \times m$ matrix defined by

$$s(i,j) = d_G(i,n) + 1, \qquad 1 \le i \le n, \quad 1 \le j \le m, \tag{16}$$

J is the matrix whose entries are all one and I is the identity matrix.

Theorem 3.1. *Let G be a connected graph on $V = \{1, 2, \dots, n\}$ and K_{m+1} the complete graph on $\{n, n+1, \dots, n+m\}$, where $n \ge 2$ and $m \ge 1$. Let $\tilde{G} = (\tilde{V}, \tilde{E}) = G \star K_{m+1}$ be the star product defined as above. If $\mathrm{QEC}(G) < 0$ and there exists $f_0 \in C(V)$ such that*

$$\mathrm{QEC}(G) = \langle f_0, D f_0 \rangle, \quad \langle f_0, f_0 \rangle = 1, \quad \langle \mathbf{1}, f_0 \rangle = 0 \tag{17}$$

and

$$f_0(n) \ne 0, \tag{18}$$

then we have

$$\mathrm{QEC}(G) < \mathrm{QEC}(G \star K_{m+1}) < 0. \tag{19}$$

Proof of the left-half of (19). For simplicity we set $\lambda_0 = \mathrm{QEC}(G)$. Then taking $f_0 \in C(V) \cong \mathbb{R}^n$ as in the above statement, we have

$$\lambda_0 = \langle f_0, D f_0 \rangle < 0, \tag{20}$$

and

$$\langle f_0, f_0 \rangle = 1, \qquad \langle \mathbf{1}, f_0 \rangle = 0. \tag{21}$$

(In fact, existence of f_0 satisfying (17) follows from the definition of QE constant. The essential assumption is (18).) On the other hand, $\mathrm{QEC}(\tilde{G})$ is given by the conditional maximum of the quadratic function:

$$\Phi = \langle \tilde{f}, \tilde{D}\tilde{f} \rangle, \quad \tilde{f} \in C(\tilde{V}) \cong \mathbb{R}^{n+m},$$

subject to

$$\langle \tilde{f}, \tilde{f} \rangle = 1, \qquad \langle \mathbf{1}, \tilde{f} \rangle = 0. \tag{22}$$

It is convenient to use new variables $(\xi, \eta) \in \mathbb{R}^m \times \mathbb{R}^m$ defined by

$$\tilde{f} = \tilde{f}_0 + \begin{bmatrix} \xi \\ \eta \end{bmatrix}, \qquad \tilde{f}_0 = \begin{bmatrix} f_0 \\ 0 \end{bmatrix}.$$

By simple algebra conditions (22) are rephrased as

$$\langle \tilde{f}, \tilde{f} \rangle = 1 \quad \Leftrightarrow \quad \langle \xi, \xi \rangle + \langle \eta, \eta \rangle + 2\langle f_0, \xi \rangle = 0, \tag{23}$$

$$\langle \mathbf{1}, \tilde{f} \rangle = 0 \quad \Leftrightarrow \quad \langle \mathbf{1}, \xi \rangle + \langle \mathbf{1}, \eta \rangle = 0. \tag{24}$$

Moreover, we have

$$\begin{aligned}\Phi = \langle \tilde{f}, \tilde{D}\tilde{f} \rangle &= \left\langle \begin{bmatrix} f_0 + \xi \\ \eta \end{bmatrix}, \begin{bmatrix} D & S \\ S^T & J - I \end{bmatrix} \begin{bmatrix} f_0 + \xi \\ \eta \end{bmatrix} \right\rangle \\ &= \lambda_0 + 2\langle f_0, D\xi \rangle + 2\langle f_0, S\eta \rangle + 2\langle \xi, S\eta \rangle + \langle \xi, D\xi \rangle + \langle \mathbf{1}, \eta \rangle^2 - \langle \eta, \eta \rangle, \end{aligned} \tag{25}$$

where we used the simple identity: $\langle \eta, J\eta \rangle = \langle \mathbf{1}, \eta \rangle^2$. Using (16) we obtain

$$\begin{aligned}\langle f_0, S\eta \rangle &= \sum_{i=1}^{n} f_0(i) S\eta(i) = \sum_{i=1}^{n} f_0(i) \sum_{j=1}^{m} (d(i,n) + 1)\eta(j) \\ &= \sum_{i=1}^{n} f_0(i)(d_G(i,n) + 1)\langle \mathbf{1}, \eta \rangle = (Df_0(n) + \langle \mathbf{1}, f_0 \rangle)\langle \mathbf{1}, \eta \rangle. \end{aligned} \tag{26}$$

Similarly,

$$\langle \xi, S\eta \rangle = (D\xi(n) + \langle \mathbf{1}, \xi \rangle)\langle \mathbf{1}, \eta \rangle. \tag{27}$$

Inserting (26) and (27) into (25), and then applying (23), (24) and (21), we obtain

$$\begin{aligned}\Phi = \Phi(\xi, \eta) = \lambda_0 &+ \langle \xi, D\xi \rangle + \langle \xi, \xi \rangle - \langle \mathbf{1}, \xi \rangle^2 \\ &+ 2\langle f_0, D\xi \rangle + 2\langle f_0, \xi \rangle - 2Df_0(n)\langle \mathbf{1}, \xi \rangle - 2D\xi(n)\langle \mathbf{1}, \xi \rangle. \end{aligned} \tag{28}$$

Thus, $\mathrm{QEC}(\tilde{G})$ coincides with the conditional maximum of $\Phi(\xi, \eta)$ subject to (23) and (24). Here note that η is implicitly contained in (28) through those conditions.

To be precise, we put

$$\mathcal{M}=\left\{(\xi,\eta)\in\mathbb{R}^n\times\mathbb{R}^m\,;\;\begin{array}{l}\langle\xi,\xi\rangle+\langle\eta,\eta\rangle+2\langle f_0,\xi\rangle=0,\\ \langle\mathbf{1},\xi\rangle+\langle\mathbf{1},\eta\rangle=0\end{array}\right\}.$$

Then we have

$$\mathrm{QEC}(\tilde{G})=\max\{\Phi(\xi,\eta)\,;\,(\xi,\eta)\in\mathcal{M}\}.$$

Since $(0,0)\in\mathcal{M}$ and $\Phi(0,0)=\lambda_0=\mathrm{QEC}(G)$, for $\mathrm{QEC}(G)<\mathrm{QEC}(\tilde{G})$ it is sufficient to show that $\Phi(\xi,\eta)$ does not attain a conditional maximum at $(\xi,\eta)=(0,0)$. We will prove this by contradiction.

Suppose that $\Phi(\xi,\eta)$ attains a conditional maximum at $(\xi,\eta)=(0,0)$. Then the directional derivative of $\Phi(\xi,\eta)$ at $(\xi,\eta)=(0,0)$ vanishes along any curve in $\mathcal{M}$ passing through $(0,0)$. For $1\le k\le n-1$ we put

$$\mathcal{N}_k=\left\{(\xi=[\xi(i)],\eta=[\eta(j)])\in\mathbb{R}^n\times\mathbb{R}^m\,;\;\begin{array}{l}\xi(i)=0\text{ except }i=k\text{ and }i=n,\\ \eta(j)=0\text{ except }j=1\end{array}\right\}$$

and

$$\mathcal{M}_k=\mathcal{M}\cap\mathcal{N}_k\,.$$

From (23) and (24) we see that $(\xi,\eta)\in\mathcal{N}_k$ belongs to $\mathcal{M}$ if and only if

$$2f_0(k)\xi(k)+2f_0(n)\xi(n)+\xi(k)^2+\xi(n)^2+\eta(1)^2=0, \tag{29}$$

$$\xi(k)+\xi(n)+\eta(1)=0. \tag{30}$$

Inserting (30) into (29), we obtain

$$\xi(k)^2+\xi(n)^2+\xi(k)\xi(n)+f_0(k)\xi(k)+f_0(n)\xi(n)=0, \tag{31}$$

which determines an ellipse of positive radius since $f_0(n)\neq 0$ by assumption. Namely, $\mathcal{M}_k$ is an ellipse in $\mathbb{R}^n\times\mathbb{R}^m$ passing through $(0,0)$.

Now consider the directional derivative of $\Phi(\xi,\eta)$ at $(\xi,\eta)=0$ along the ellipse $\mathcal{M}_k$. From (31) we obtain easily that

$$\left.\frac{d\xi(n)}{d\xi(k)}\right|_{(\xi(k),\xi(n))=(0,0)}=-\left.\frac{f_0(k)+2\xi(k)+\xi(n)}{f_0(n)+\xi(k)+2\xi(n)}\right|_{(\xi(k),\xi(n))=(0,0)}=-\frac{f_0(k)}{f_0(n)}.$$

On the other hand, inserting (29) and (30) into (28), we see that $\Phi=\Phi(\xi,\eta)$ on $\mathcal{M}_k$ becomes

$$\begin{aligned}\Phi=\Phi(\xi(k),\xi(n))&=\lambda_0-2d(n,k)\xi(k)^2-2\xi(k)\xi(n)\\&\qquad+2(f_0(k)+Df_0(k)-Df_0(n))\xi(k)+2f_0(n)\xi(n).\end{aligned}$$

Then again by simple calculus, we come to

$$\left.\frac{d\Phi}{d\xi(k)}\right|_{(\xi(k),\xi(n))=(0,0)}=2Df_0(k)-2Df_0(n). \tag{32}$$

Since $d\Phi/d\xi(k)$ at $\xi = 0$ vanishes for all $1 \le k \le n-1$ by assumption, it follows from (32) that $Df_0(k) = Df_0(n)$ for all $1 \le k \le n-1$. Hence $Df_0 = Df_0(n)\mathbf{1}$ and we come to

$$\lambda_0 = \langle f_0, Df_0 \rangle = Df_0(n)\langle f_0, \mathbf{1} \rangle = 0,$$

which is in contradiction to $\lambda_0 = \mathrm{QEC}(G) < 0$. □

Proposition 3.1. *Let G_1 and G_2 be connected graphs with $\mathrm{QEC}(G_1) < 0$ and $\mathrm{QEC}(G_2) < 0$. Then*

$$\mathrm{QEC}(G_1 \star G_2) \le \left(\frac{1}{\mathrm{QEC}(G_1)} + \frac{1}{\mathrm{QEC}(G_2)} \right)^{-1} < 0. \tag{33}$$

For the proof see [14, Section 4], where a more precise estimate is obtained.

Proof of the right-half of (19). Note that $\mathrm{QEC}(K_{m+1}) = -1$ for all $m \ge 1$. It then follows immediately from Proposition 3.1 that

$$\mathrm{QEC}(G \star K_m) \le \left(\frac{1}{\mathrm{QEC}(G)} + \frac{1}{-1} \right)^{-1} = \frac{\mathrm{QEC}(G)}{1 - \mathrm{QEC}(G)} < 0.$$

Here condition (18) is not necessary. □

Remark 3.1. For the strict inequality of the left-half of (19) condition (18) is necessary. We give a simple example. Consider the graph G on five verices and $\tilde{G} = G \star K_2$ on six vertices as is illustrated in Figure 2. By a direct computation we easily obtain

$$\mathrm{QEC}(G) = \mathrm{QEC}(\tilde{G}) = -\frac{2}{2+\sqrt{2}}\,.$$

In fact, $\mathrm{QEC}(G)$ is attained by

$$f_0 = c \begin{bmatrix} \pm 1 \\ \mp 1 \\ \pm(\sqrt{2}+1) \\ \mp(\sqrt{2}+1) \\ 0 \end{bmatrix}, \qquad c = \sqrt{\frac{2-\sqrt{2}}{8}}.$$

Indeed, $f_0(5) = 0$ and condition (18) is fulfilled. More examples will appear in Subsection 4.5. While, it is not clear whether $\mathrm{QEC}(G) = \mathrm{QEC}(\tilde{G})$ follows from $f_0(n) = 0$.

3.2. QE Constants of Paths

For $n \ge 1$, let P_n be the path on $\{1, 2, \dots, n\}$. Since P_n is isometrically embedded in P_{n+1}, we have

$$\mathrm{QEC}(P_n) \le \mathrm{QEC}(P_{n+1}), \qquad n \ge 2.$$

In this section, we prove that the above inequality is strict.

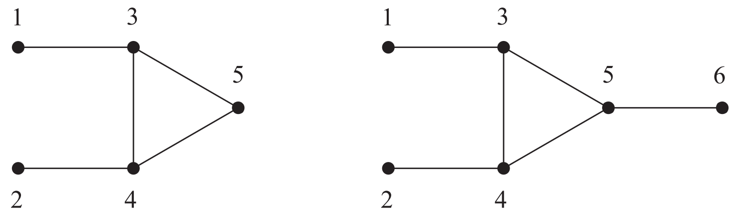

Figure 2. An example of $f_0(5) = 0$.

Theorem 3.2. *For* $n \geq 2$ *we have* $\mathrm{QEC}(P_n) < \mathrm{QEC}(P_{n+1})$.

Proof. The distance matrix of P_n is given by $D = [d(i,j)]$ with $d(i,j) = |i-j|$, $1 \leq i,j \leq n$. According to the general method described in Subsection 2.2 let $\mathcal{S}$ be the set of $(f, \lambda, \mu) \in \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}$ such that

$$(D - \lambda)f = \frac{\mu}{2}\,\mathbf{1}, \tag{34}$$

$$\langle f, f \rangle = 1, \tag{35}$$

$$\langle \mathbf{1}, f \rangle = 0. \tag{36}$$

Then $\lambda_0 = \mathrm{QEC}(P_n)$ is the maximum of $\lambda \in \mathbb{R}$ such that $(f, \lambda, \mu) \in \mathcal{S}$ for some $f \in \mathbb{R}^n$ and $\mu \in \mathbb{R}$. It is readily known that $\lambda_0 < 0$. By virtue of Theorem 3.1 it is sufficient to show that there exists $(f_0 = [f_0(i)], \lambda_0, \mu_0) \in \mathcal{S}$ such that $f_0(n) \neq 0$.

In fact, we will prove a slightly stronger result: for any $(f = [f(i)], \lambda, \mu) \in \mathcal{S}$ we have $f(n) \neq 0$. First assume that $(f, \lambda, \mu) \in \mathcal{S}$ fulfills

$$f(j) = 0 \quad \text{for} \quad k \leq j \leq n, \tag{37}$$

where $2 \leq k \leq n$. We will derive $f(k-1) = 0$. The k-th coordinate of (34) is given by

$$\sum_{j=1}^{n} |k-j| f(j) - \lambda f(k) = \frac{\mu}{2} \tag{38}$$

and by assumption (37) we have

$$\sum_{j=1}^{k-1} (k-j) f(j) - \lambda f(k) = \frac{\mu}{2}\,. \tag{39}$$

Similarly, looking at the $(k-1)$-th coordinate of (34), we obtain

$$\sum_{j=1}^{k-1} (k-1-j) f(j) - \lambda f(k-1) = \frac{\mu}{2}\,. \tag{40}$$

On the other hand, by (36) and (37) we have

$$\sum_{j=1}^{k-1} f(j) = 0.$$

Then (40) becomes

$$\sum_{j=1}^{k-1} (k-j)f(j) - \lambda f(k-1) = \frac{\mu}{2}\,. \tag{41}$$

Comparing (39) and (41), we obtain

$$\lambda(f(k-1) - f(k)) = 0.$$

Since $\lambda \le \lambda_0 < 0$, we obtain $f(k-1) = f(k) = 0$ as desired. Thus, by induction we see that $f(n) = 0$ implies that $f(j) = 0$ for all $1 \le j \le n$, which is in contradiction to condition (35). Consequently, $f(n) \neq 0$ for any $(f, \lambda, \mu) \in \mathcal{S}$. □

Proposition 3.2. *We have*

$$\lim_{n\to\infty} \mathrm{QEC}(P_n) = -\frac{1}{2}\,.$$

For the proof see [14, Section 5], where a precise estimate of $\mathrm{QEC}(P_n)$ from below is obtained.

4. Classification of Graphs Along $\mathrm{QEC}(P_n)$

4.1. Formulation of Problem

Combining Theorem 3.2 and Proposition 3.2, we come to

$$\mathrm{QEC}(P_2) < \mathrm{QEC}(P_3) < \cdots < \mathrm{QEC}(P_n) < \mathrm{QEC}(P_{n+1}) < \cdots \to -\frac{1}{2}. \tag{42}$$

In fact, the first few are given as follows:

$$\begin{aligned}
\mathrm{QEC}(P_2) &= -1, \\
\mathrm{QEC}(P_3) &= -\frac{2}{3} = -0.6666\cdots, \\
\mathrm{QEC}(P_4) &= -\frac{2}{2+\sqrt{2}} = -(2-\sqrt{2}) = -0.5857\cdots, \\
\mathrm{QEC}(P_5) &= -\frac{4}{5+\sqrt{5}} = -\frac{5-\sqrt{5}}{5} = -0.5527\cdots, \\
\mathrm{QEC}(P_6) &= -\frac{2}{2+\sqrt{3}} = -(4-2\sqrt{3}) = -0.5358\cdots.
\end{aligned}$$

A closed formula for $\mathrm{QEC}(P_n)$ is not known.

Our main interest along (42) is to characterize the family of graphs G satisfying

$$\mathrm{QEC}(P_n) \le \mathrm{QEC}(G) < \mathrm{QEC}(P_{n+1}), \qquad n \ge 2, \tag{43}$$

in terms of geometric or combinatorial properties of graphs. We are also interested in the graphs G satisfying

$$\mathrm{QEC}(G) < -\frac{1}{2}\,. \tag{44}$$

We first recall the following simple fact mentioned in Corollary 2.2 (2).

Proposition 4.1. *Let* $n \ge 2$. *If* $\mathrm{QEC}(G) < \mathrm{QEC}(P_{n+1})$, *then* $\mathrm{diam}(G) \le n-1$.

Next we provide simple criteria for (44) in terms of forbidden subgraphs. Let $K_4\backslash\{e\}$ denote the *diamond*, that is, the graph obtained by deleting one edge from the complete graph K_4, see Figure 3. Let $K_{m,n}$ denote the complete bipartite graph with two parts of m and n vertices. In particular, $K_{1,n}$ is called a *star* and $K_{1,3}$ a *claw*, see Figure 3.

Figure 3. $K_4\backslash\{e\}$ (diamond) and $K_{1,3}$ (claw).

Proposition 4.2. *If a connected graph G contains an induced subgraph isomorphic to a diamond $K_4\backslash\{e\}$ or a claw $K_{1,3}$, then* $\mathrm{QEC}(G) \ge -1/2$.

Proof. It is easily verified [18, Section 5] that

$$\mathrm{QEC}(K_4\backslash\{e\}) = \mathrm{QEC}(K_{1,3}) = -\frac{1}{2}\,.$$

Moreover we have $\mathrm{diam}(K_4\backslash K_2) = \mathrm{diam}(K_{1,3}) = 2$. It then follows from Proposition 2.3 that $\mathrm{QEC}(G) \ge -1/2$. □

Proposition 4.3. *If a connected graph G contains an induced subgraph isomorphic to the cycle C_4, then* $\mathrm{QEC}(G) \ge 0$. *If G contains an induced subgraph isomorphic to C_5, then*

$$\mathrm{QEC}(G) \ge -\frac{2}{3+\sqrt{5}} = -0.3819\ldots.$$

Proof. We note that

$$\mathrm{QEC}(C_4) = 0, \qquad \mathrm{QEC}(C_5) = -\frac{2}{3+\sqrt{5}},$$

see also (6). Then the assertion follows in a similar manner as in the proof of Proposition 4.2. □

The following result is immediate from Propositions 4.2 and 4.3.

Corollary 4.1 (forbidden subgraphs)**.** *Any graph with* $\mathrm{QEC}(G) < -1/2$ *does not contain an induced subgraph isomorphic to a diamond* $K_4\backslash\{e\}$*, a claw* $K_{1,3}$*, a cycle* C_4*, nor* C_5*. In short, any graph with* $\mathrm{QEC}(G) < -1/2$ *is diamond-free, claw-free,* C_4*-free and* C_5*-free.*

Remark 4.1. As an immediate consequence from Corollary 4.1, the family of graphs with $\mathrm{QEC}(G) < -1/2$ forms a subfamily of the claw-free graphs. On the other hand, claw-free graphs have been actively studied with various classifications, see for instance [7]. It would be interesting to revisit the classification of claw-free graphs along with $\mathrm{QEC}(P_n)$.

4.2. Determining the class $\mathrm{QEC}(P_2) \le \mathrm{QEC}(G) < \mathrm{QEC}(P_3)$

Theorem 4.1. *For a connected graph* G *the inequality*

$$\mathrm{QEC}(P_2) \le \mathrm{QEC}(G) < \mathrm{QEC}(P_3) \tag{45}$$

holds if and only if $G = K_n$ *for some* $n \ge 2$*. Moreover,* $\mathrm{QEC}(P_2) = \mathrm{QEC}(K_n)$ *for all* $n \ge 2$*. Therefore, there is no graph* G *such that* $\mathrm{QEC}(P_2) < \mathrm{QEC}(G) < \mathrm{QEC}(P_3)$*.*

Proof. Suppose that a graph G satisfies (45). Then by Proposition 4.1, we have $\mathrm{diam}(G) = 1$, which means that G is a complete graph. On the other hand, it is known that $\mathrm{QEC}(K_n) = -1 = \mathrm{QEC}(P_2)$ for all $n \ge 2$. The assertion is then obvious. □

4.3. Calculating $\mathrm{QEC}(K_n \star K_m)$

We consider the star product of two complete graphs K_n and K_m, see Figure 4. To be precise, let $n \ge 1$ and $m \ge 2$, and consider the graphs $\tilde{G} = (\tilde{V}, \tilde{E})$, where

$$\tilde{V} = \{1, 2, \dots, n\} \cup \{n, n+1, \dots, n+m-1\}$$

and

$$\tilde{E} = \{\{i, j\}\,;\, 1 \le i < j \le n\} \cup \{\{i, j\}\,;\, n \le i < j \le n+m-1\}.$$

Obviously, we have $\tilde{G} = K_n \star K_m$, where the induced subgraphs spanned by $\{1, 2, \dots, n\}$ and by $\{n, n+1, \dots, n+m-1\}$ are the complete graphs K_n and K_m, respectively.

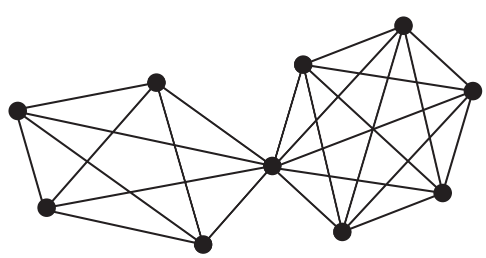

Figure 4. $K_n \star K_m$ $(n = 5, m = 6)$.

Let $\tilde{D}$ be the distance matrix of $\tilde{G} = K_n \star K_m$. It is convenient to write $\tilde{D}$ in the block matrices:

$$\tilde{D} = \left[\begin{array}{c|c} J-I & S \\ \hline S^T & J-I \end{array}\right], \qquad S = \begin{bmatrix} 2 & \cdots & 2 \\ \vdots & & \vdots \\ 2 & \cdots & 2 \\ 1 & \cdots & 1 \end{bmatrix}, \tag{46}$$

where S is an $n \times (m-1)$ matrix. The QE constant $\mathrm{QEC}(\tilde{G})$ is the conditional maximum of

$$\Phi = \langle \tilde{f}, \tilde{D}\tilde{f} \rangle, \qquad \tilde{f} \in C(\tilde{V}), \tag{47}$$

subject to

$$\langle \tilde{f}, \tilde{f} \rangle = 1, \qquad \langle \mathbf{1}, \tilde{f} \rangle = 0.$$

According to the block diagonal expression (46), we write $\tilde{f} = [f \;\; g]^T$, where $f \in \mathbb{R}^n$, $g \in \mathbb{R}^{m-1}$. Then (47) becomes

$$\begin{aligned} \Phi = \Phi(f,g) &= \left\langle \begin{bmatrix} f \\ g \end{bmatrix}, \begin{bmatrix} J-I & S \\ S^T & J-I \end{bmatrix} \begin{bmatrix} f \\ g \end{bmatrix}, \right\rangle \\ &= \langle 1, f \rangle^2 + \langle 1, g \rangle^2 - \langle f, f \rangle - \langle g, g \rangle + 4\langle \mathbf{1}, f \rangle \langle \mathbf{1}, g \rangle - 2f_n \langle \mathbf{1}, g \rangle, \end{aligned}$$

where we used

$$Sg = \langle \mathbf{1}, g \rangle [2\; 2 \cdots \; 2\; 1]^T.$$

Define

$$F(f,g,\lambda,\mu) = \Phi(f,g) - \lambda(\langle f, f \rangle + \langle g, g \rangle - 1) - \mu(\langle \mathbf{1}, f \rangle + \langle \mathbf{1}, g \rangle)$$

and let $\mathcal{S}$ be the set of its stationary points $(f,g,\lambda,\mu) \in \mathbb{R}^n \times \mathbb{R}^{m-1} \times \mathbb{R} \times \mathbb{R}$, that is the solutions to

$$\frac{\partial F}{\partial f_i} = \frac{\partial F}{\partial g_j} = \frac{\partial F}{\partial \lambda} = \frac{\partial F}{\partial \mu} = 0, \quad 1 \le i \le n, \;\; 1 \le j \le m-1. \tag{48}$$

Keeping in mind that $-1 < \mathrm{QEC}(\tilde{G}) < 0$ unless $m = 1$ or $n = 1$, we find after simple calculus that the maximum of λ appearing in the solution is

$$\lambda = \frac{-mn + \sqrt{mn(m-1)(n-1)}}{m+n-1} = -\frac{1}{1 + \sqrt{\left(1 - \dfrac{1}{m}\right)\left(1 - \dfrac{1}{n}\right)}},$$

which coincides with $\mathrm{QEC}(\tilde{G})$ by the general theory mentioned in Subsection 2.2. We have thus obtained the following result.

Proposition 4.4. *For $m \ge 1$ and $n \ge 1$ with $m + n \ge 3$ with we have*

$$\mathrm{QEC}(K_n \star K_m) = -\frac{1}{1 + \sqrt{\left(1 - \dfrac{1}{m}\right)\left(1 - \dfrac{1}{n}\right)}}.$$

Corollary 4.2. *We have*

$$\begin{aligned}\mathrm{QEC}(P_3) = \mathrm{QEC}(K_2 \star K_2) < \mathrm{QEC}(K_3 \star K_2) < \cdots \\ \cdots < \mathrm{QEC}(K_n \star K_2) < \cdots \to \mathrm{QEC}(P_4) = -\frac{2}{2+\sqrt{2}}.\end{aligned} \tag{49}$$

Proof. By Proposition 4.4 we have

$$\mathrm{QEC}(K_n \star K_2) = -\frac{2}{2+\sqrt{2\Big(1-\dfrac{1}{n}\Big)}}\,, \quad n \geq 1,$$

from which the assertion follows immediately. □

Corollary 4.3. *Let $m \geq 1$ and $n \geq 1$ with $m+n \geq 3$. Then $\mathrm{QEC}(K_n \star K_m) < \mathrm{QEC}(P_4)$ if and only if one of the following conditions is satisfied:*

(i) $m = 2$ *and* $n \geq 1$*;*
(ii) $m \geq 1$ *and* $n = 2$*;*
(iii) $m = n = 3$.

Proof. The inequality $\mathrm{QEC}(K_n \star K_m) < \mathrm{QEC}(P_4)$ is equivalent to

$$-\frac{1}{1+\sqrt{\Big(1-\dfrac{1}{m}\Big)\Big(1-\dfrac{1}{n}\Big)}} < -\frac{2}{2+\sqrt{2}}\,,$$

of which integer solutions are obtained easily by simple algebra. □

Corollary 4.4. *Let $m \geq 1$ and $n \geq 1$ with $m+n \geq 3$. Then*

$$\mathrm{QEC}(P_3) \leq \mathrm{QEC}(K_n \star K_m) < \mathrm{QEC}(P_4) \tag{50}$$

holds if and only if one of the following conditions is satisfied:

(i) $m = 2$ *and* $n \geq 2$*;*
(ii) $m \geq 2$ *and* $n = 2$*;*
(iii) $m = n = 3$.

The equality in (50) *occurs only when $m = n = 2$.*

4.4. Determining the class $\mathrm{QEC}(P_3) \leq \mathrm{QEC}(G) < \mathrm{QEC}(P_4)$

This subsection is devoted to the proof of the following result.

Theorem 4.2. *A finite connected graph G fulfills the inequality*

$$\mathrm{QEC}(P_3) \le \mathrm{QEC}(G) < \mathrm{QEC}(P_4) \tag{51}$$

if and only if G is a star product $K_n \star K_2$ with $n \ge 2$ or $K_3 \star K_3$. Moreover,

$$\mathrm{QEC}(K_n \star K_2) = -\frac{2}{2 + \sqrt{2\Big(1 - \dfrac{1}{n}\Big)}}\,,$$

$$\mathrm{QEC}(K_3 \star K_3) = -\frac{3}{5}\,.$$

In particular, $\mathrm{QEC}(G) = \mathrm{QEC}(P_3)$ *if and only if* $G = P_3 = K_2 \star K_2$.

Lemma 4.1. *If a connected graph $G = (V, E)$ satisfies* (51)*, we have $|V| \ge 3$ and* $\mathrm{diam}(G) = 2$.

Proof. It follows from Corollary 2.2 that $\mathrm{diam}(G) \le 2$. If $\mathrm{diam}(G) = 1$, then G is a complete graph and $\mathrm{QEC}(G) = -1$, which does not satisfy (51). Hence, necessarily $\mathrm{diam}(G) = 2$ and $|V| \ge 3$. □

In general, a *clique* of G is an induced subgraph of G which is isomorphic to a complete graph. A clique $K = (W, F)$ is called *maximal* if there is no clique containing K properly. A maximal clique $K = (W, F)$ is called *largest* or *maximum* if there is no clique on $|W| + 1$ vertices. Clearly, any graph contains a largest clique.

Lemma 4.2. *Let $G = (V, E)$ be a connected graph satisfying* (51)*. If $K = (W, F)$ is a maximal clique of G, we have $W \ne V$ and $|W| \ge 2$.*

Proof. Since G is not a complete graph by Lemma 4.1, we have $W \ne V$. That $|W| \ge 2$ follows from $|V| \ge 3$. □

Lemma 4.3. *Let $G = (V, E)$ be a connected graph with $|V| \ge 2$ and $\mathrm{QEC}(G) < -1/2$, and $K = (W, F)$ a maximal clique. Then for any pair $a \in V \backslash W$ and $a' \in W$ with $a \sim a'$ we have $\{x \in W\,;\, x \sim a\} = \{a'\}$.*

Proof. (Note that the assertion is trivial if $W = V$.) Given a pair $a \in V \backslash W$ and $a' \in W$ with $a \sim a'$, we set $s = |\{x \in W\,;\, x \sim a\}|$. Obviously, $1 \le s < |W|$. We will show by contradiction that $s = 1$. Suppose that $s \ge 2$. Then there exist three distinct vertices $x_1, x_2, y \in W$ such that $a \sim x_1$, $a \sim x_2$ and $a \not\sim y$. Note that the induced subgraph spanned by $\{a, x_1, x_2, y\}$ is isomorphic to a diamond $K_4 \backslash \{e\}$. It then follows immediately from Proposition 4.2 that $\mathrm{QEC}(G) \ge -1/2$, which is in contradiction to the assumption $\mathrm{QEC}(G) < -1/2$. □

Lemma 4.4. *Let $G = (V, E)$ be a connected graph satisfying* (51) *and $K = (W, F)$ a maximal clique of G. For $a, b \in V \backslash W$ and $a', b' \in W$, if $a \sim a'$ and $b \sim b'$, then $a' = b'$.*

Proof. If $a = b$ the assertion follows immediately from Lemma 4.3. We consider the case of $a \neq b$. To prove the assertion by contradiction, we assume that $a' \neq b'$. Since $d(a,b) \le \mathrm{diam}(G) = 2$, we have two cases: $d(a,b) = 1$ or $d(a,b) = 2$.

Suppose first that $d(a,b) = 1$, that is, $a \sim b$. Then the induced subgraph spanned by $\{a, a', b', b\}$ is isomorphic to C_4, which is a forbidden subgraph by Corollary 4.1. Hence $d(a,b) = 1$ does not happen.

Suppose next that $d(a,b) = 2$. Then there exists $c \in V$ such that $a \sim c \sim b$. Since $a \not\sim b'$ and $b \not\sim a'$ by Lemma 4.3, we have $c \neq a', b'$ and $c \notin W$. There are four cases:

(i) $c \not\sim a'$ and $c \not\sim b'$. The induced subgraph spanned by $\{a, a', b', b, c\}$ is isomorphic to C_5, which is a forbidden subgraph by Corollary 4.1.

(ii) $c \not\sim a'$ and $c \sim b'$. The induced subgraph spanned by $\{a, a', b', c\}$ is isomorphic to C_4, which is a forbidden subgraph by Corollary 4.1.

(iii) $c \sim a'$ and $c \not\sim b'$. This case is similar to (ii).

(iv) $c \sim a'$ and $c \sim b'$. This does not happen by virtue of Lemma 4.3.

In any case we come to contradiction and the proof is completed. □

Proof of Theorem 4.2. Let $G = (V,E)$ be a connected graph satisfying (51) $K = (W,F)$ be a largest clique with $m = |W|$. Note that $V \neq W$ and $m \geq 2$ by Lemma 4.2. Now divide $V \backslash W$ into two subsets:

$$V \backslash W = U_1 \cup U_2\,,$$

where U_1 is the set of vertices $a \in V \backslash W$ which are directly connected to vertices in W, and U_2 the rest, see Figure 5. Obviously, $U_1 \neq \emptyset$. Moreover, by Lemma 4.4 there exists a unique $a' \in W$ such that $a \sim a'$ for all $a \in U_1$.

We first prove that $U_2 = \emptyset$. Suppose otherwise. Take $x \in W$ with $x \neq a'$ and $y \in U_2$. Then we have $d(x,y) \geq 3$, which is in contradiction to $\mathrm{diam}(G) = 2$.

We next prove that any pair of vertices $a, b \in U_1$, $a \neq b$, are connected by an edge. Suppose otherwise. Take $x \in W$ with $x \neq a'$ and consider the induced subgraph spanned by $\{x, a', a, b\}$ is isomorphic to $K_{1,3}$, which is a forbidden subgraph by Corollary 4.1.

Consequently, The induced subgraph spanned by U_1 is a complete graph on $|U_1| \geq 1$ vertices. Hence G is necessarily a star product of two complete graphs: $G = K_m \star K_{|U_1|+1}$. Then the assertion follows from Corollary 4.4. □

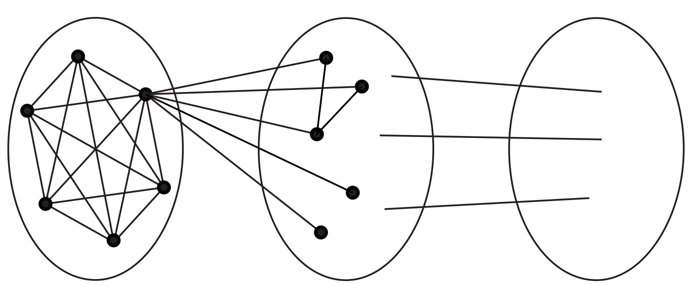

Figure 5. $V = W \cup U_1 \cup U_2$.

4.5. Bearded Complete Graphs $BK_{n,m}$

We are also interested in characterization of a graph G satisfying

$$\mathrm{QEC}(G) = \mathrm{QEC}(P_4) = -\frac{2}{2+\sqrt{2}}\,.$$

Below we give a partial answer.

Let $1 \le m \le n$. Consider a graph on

$$V = \{1, 2, \dots, n\} \cup \{n+1, \dots, n+m\}$$

with edge set

$$E = \{\{i, j\}\,;\, 1 \le i < j \le n\} \cup \{\{i, n+i\}\,;\, 1 \le i \le m\}.$$

The induced subgraph spanned by $\{1, 2, \dots, n\}$ is the complete graph K_n. We write $G = BK_{n,m}$ and call it a *bearded complete graph*.

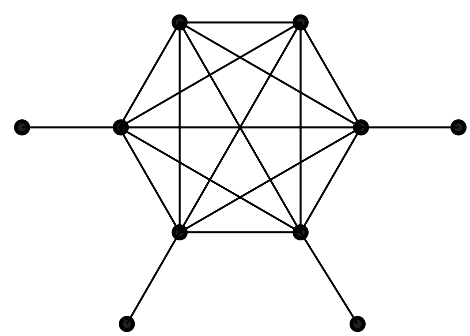

Figure 6. $BK_{n,m}$ $(n = 6, m = 4)$.

The distance matrix D of $G = BK_{n,m}$ is written in the block matrices:

$$D = \left[\begin{array}{c|c|c} J-I & J & 2J-I \\ \hline J & J-I & 2J \\ \hline 2J-I & 2J & 3J-3I \end{array}\right], \tag{52}$$

where the diagonal matrices are of $m \times m$, $(n-m) \times (n-m)$ and $m \times m$, in order.

For $m = n = 1$ by definition $BK_{1,1} = K_2$. Hence

$$\mathrm{QEC}(BK_{1,1}) = -1.$$

For $m = 1$ and $n \geq 2$ we have $BK_{n,1} = K_n \star K_2 = K_n \wedge K_{1,1}$. It is already known that

$$\mathrm{QEC}(BK_{n,1}) = -\frac{2}{2 + \sqrt{2\Big(1 - \dfrac{1}{n}\Big)}}\,.$$

The above formula is valid for $n = 1$.

Theorem 4.3. *Let* $2 \leq m \leq n$. *Then*

$$\mathrm{QEC}(BK_{n,m}) = -\frac{2}{2+\sqrt{2}} = -(2-\sqrt{2}) = \mathrm{QEC}(P_4).$$

Proof. According to the expression (52) in block diagonal form, the quadratic function $\Phi = \langle \tilde{f}, D\tilde{f} \rangle$ becomes

$$\begin{aligned}
\Phi &= \left\langle \begin{bmatrix} f \\ g \\ h \end{bmatrix}, \begin{bmatrix} J-I & J & 2J-I \\ J & J-I & 2J \\ 2J-I & 2J & 3J-3I \end{bmatrix}, \begin{bmatrix} f \\ g \\ h \end{bmatrix} \right\rangle \\
&= \langle \mathbf{1}, f\rangle^2 + \langle \mathbf{1}, g\rangle^2 + 3\langle \mathbf{1}, h\rangle^2 - \langle f, f\rangle - \langle g, g\rangle - 3\langle h, h\rangle \\
&\qquad + 2\langle \mathbf{1}, f\rangle\langle \mathbf{1}, g\rangle + 4\langle \mathbf{1}, f\rangle\langle \mathbf{1}, h\rangle + 4\langle \mathbf{1}, g\rangle\langle \mathbf{1}, h\rangle - 2\langle f, h\rangle,
\end{aligned}$$

where

$$\tilde{f} = \begin{bmatrix} f \\ g \\ h \end{bmatrix}, \qquad f \in \mathbb{R}^m, \quad g \in \mathbb{R}^{n-m}, \quad h \in \mathbb{R}^m.$$

We then consider the stationary points of

$$\begin{aligned}
F(f, g, h, \lambda, \mu) = \Phi &- \lambda(\langle f, f\rangle + \langle g, g\rangle + \langle h, h\rangle - 1) \\
&- \mu(\langle \mathbf{1}, f\rangle + \langle \mathbf{1}, g\rangle + \langle \mathbf{1}, h\rangle).
\end{aligned}$$

After simple calculus we see that the largest λ appearing in the stationary points of $F(f, g, h, \lambda, \mu)$ is given by

$$\lambda = -(2-\sqrt{2}),$$

with

$$\langle \mathbf{1}, f\rangle = 0, \quad \langle f, f\rangle = \frac{2+\sqrt{2}}{4}, \quad g = 0, \quad h = -(\lambda+1)f, \quad \mu = 0.$$

Indeed, by virtue of the condition $m \geq 2$, we may choose $f \in \mathbb{R}^m$ satisfying the first two conditions. □

Note

The QE constants of graphs on n vertices with $n \leq 5$ are listed in [18], in which the QE constant of the graph No. 12 on $n = 5$ verices needs correction:

$$\text{for} \quad -\frac{4}{5+\sqrt{5}} \qquad \text{read} \qquad -\frac{4}{5+\sqrt{15}}$$

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