Chapter 4

Complete Bipartite Graphs with Self-loops

We start this chapter with a very well-known result from matrix theory.

$$\text{If } Spec(M) \subseteq \mathbb{Z}, \text{ then } Spec(M + rI) \subseteq \mathbb{Z}, \text{ for any } r \in \mathbb{Z}.$$

However, the above result is still unknown if we replace the matrix I with any non-zero $(0,1)$-diagonal matrix. In this chapter, we answer this question when M is the signless Laplacian matrix of some special graph classes.

In Chapters 2-4, we considered only simple graph. In this chapter, we focus on graphs having self-loops.

Let G^H be a graph obtained from G by adding a self-loop to each vertices of $H \subseteq V(G)$. Graphs with self-loops (representing heteroatoms) are of evident chemical significance, and were much studied in the past, including their spectral properties [1, 19, 34]. Recently, in 2022 [21], the authors gave a bound of the adjacency energy of G^H in terms of $|E(G)|$, $|V(G)|$ and $|H|$. It is also interesting to see that the adjacency energy of G^H and $G^{V(G)\setminus H}$ are equal. In the same article, the authors gave a conjecture stating that the energy of G^H is strictly greater than the energy of G when H is a non-empty proper subset of $V(G)$. However, in 2023 [27], the conjecture was disproved. In [37], the characteristic polynomials of the graph with loops were studied. For results related to graphs with self-loops, see [2, 26]. Moreover, the energy of graphs has a direct connection with the eigenvalues, and the graphs with integral Q-spectrum are of high interest now, see [29, 30, 35]. This motivates us to observe how the addition of self-loops affects the spectrum of a Q-integral graph, that is, whether the graph remains Q-integral after the addition.

Note that, the addition of a self-loop at vertex v in G increases the degree of v by 2, and the (v, v)-th entry in the adjacency matrix of new graph becomes 1. The adjacency matrix $A(G^H) = (a_{uv})$ of G^H is of order $|V(G^H)| = |V(G)|$ whose rows and columns correspond to $V(G^H)$ and is defined by

$$a_{uv} = \begin{cases} 1 & \text{if } \ uv \in E(G^H) \\ 0 & \text{otherwise.} \end{cases}$$

The diagonal matrix $D(G^H) = (d_{G^H}(v))$ of vertex degrees is given by

$$d_{G^H}(v) = \begin{cases} d_G(v) & \text{if } \ v \notin H \\ d_G(v) + 2 & \text{if } \ v \in H. \end{cases}$$

Thus, $Q(G^H) = Q(G) + 3D'$, where D' is a $(0,1)$-diagonal matrix with $D'_{vv} = 0$ if $v \notin H$ and $D'_{vv} = 1$ otherwise. In this chapter, we discuss when $Spec(Q(G^H))$ contains only integer values. Now, we give some results on $Q(G^H)$.

Proposition 4.1. *If G is a simple undirected graph and $H \subseteq V(G)$, then the signless Laplacian $Q(G^H)$ is positive semidefinite.*

Proof. Suppose y is any non-zero vector and y^T is the transpose of y. Let $Q(G^H) = Q(G) + 3D'$, for some $(0,1)$-diagonal matrix D'. Since $Q(G)$ is positive semidefinite, we have $y^T Q(G^H) y = y^T Q(G) y + 3y^T D' y \geq 0$. □

Remark 4.2. Suppose G is a simple Q-integral graph. When $H = \emptyset$, we have $G^H = G$ and when $H = V(G)$, then $Q(G^H) = Q(G) + 3I$. Therefore, G^H is Q-integral if $H \in \{\emptyset, V(G)\}$.

In view of the above remark, we focus on the non-empty proper subset H of $V(G)$.

Particularly, we discuss the Q-integrality of the complete bipartite graph $K_{q,p}$ containing self-loops when $q = 1$ and $q = p$. Let $V(K_{q,p}) = V_1 \cup V_2$ such that $V_1 \cap V_2 = \emptyset$ and $|V_1| = q, |V_2| = p$. We use $K_{q,p}^{m,k}$ to denote the graph $K_{q,p}^H$ by adding m-self-loops to any of m-distinct vertices of V_1 and k-self-loops to any of the k-distinct vertices of V_2, see Figure 4.1. Clearly, $0 \leq m \leq q$ and $0 \leq k \leq p$. Note that $H = H_1 \cup H_2$ where $H_i \subseteq V_i (i = 1, 2)$ and $|H_1| = m$, $|H_2| = k$.

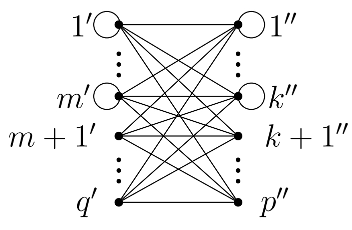
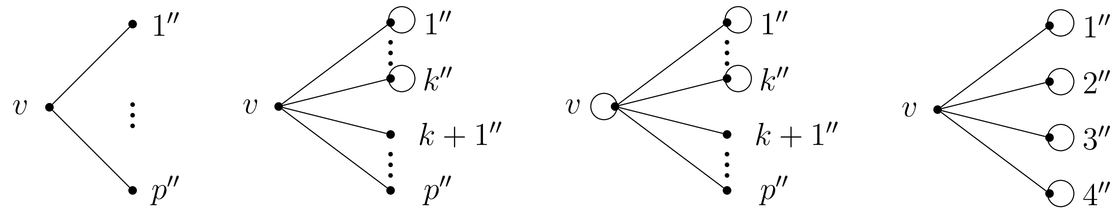


FIGURE 4.1: The graph $K_{q,p}^{m,k}$.

4.1 Star Graph

We start with the star graph $K_{1,p}$. We call the vertex of degree p in $K_{1,p}$ as central vertex. Let $V(K_{1,p}) = \{v, 1'', \ldots, p''\}$ and degree of v be p. Recall that $\lambda^{(r)}$ denotes the eigenvalue λ with algebraic multiplicity r.



(a) $K_{1,p}$ (b) $K_{1,p}^{0,k}$ (c) $K_{1,p}^{1,k}$ (d) $K_{1,4}^{0,4}$

FIGURE 4.2: Star graph $K_{1,p}$ and star graphs with self-loops.

Theorem 4.3. *Let $\emptyset \neq H \subset V(K_{1,p})$ with $|H| = m + k$, where m self-loop is added to the central vertex and k-self-loops are added to k-pendant vertices of $K_{1,p}$, for $m \in \{0, 1\}$ and $0 \leq k \leq p$. Then the following hold.*

(i) *Spec*$(K_{1,p}^H) = \{1^{(p-1)}, \frac{p+4\pm\sqrt{p^2+8p+4}}{2}\}$ *if* $k = 0$.

(ii) *Spec*$(K_{1,p}^H) = \{4^{(p-1)}, \frac{p+4\pm\sqrt{p^2-4p+16}}{2}\}$ *if* $k = p$.

(iii) $\{4^{(k-1)}, 1^{(p-k-1)}\} \subset$ *Spec*$(K_{1,p}^H)$ *if* $1 \leq k < p$.

(iv) $K_{1,p}^H$ *is Q-integral if and only if* $K_{1,p}^H = K_{1,4}^{0,4}$.

Proof. Without loss of generality, suppose self-loops are added to the k-pendant vertices $\{1'', \ldots, k''\}$ of $V(K_{1,p})$. Let m self-loop be added to the central vertex of $K_{1,p}$, where $m \in \{0, 1\}$. Then the signless Laplacian $Q(K_{1,p}^H)$ corresponding to the vertex set $\{v, 1'', \ldots, p''\}$ is

$$Q(K_{1,p}^H) = \begin{pmatrix} p + 3m & \mathrm{J}_{1\times p} \\ \mathrm{J}_{p\times 1} & B \end{pmatrix}, \text{ where } B = \begin{pmatrix} 4I_k & \mathrm{O} \\ \mathrm{O} & I_{p-k} \end{pmatrix}.$$

Using Theorem 1.1, we get the following characteristic polynomial of $Q(K_{1,p}^H)$

$$\mathcal{P}_Q(z) = (z-4)^{k-1}(z-1)^{p-k-1}\{(z-p-3m)(z-4)(z-1)-k(z-1)-(p-k)(z-4)\}.$$

If $k = 0$, then $H = \{v\}$ as $H \neq \emptyset$, and so, $m = 1$. For $k = p$, we have $H = V(K_{1,p}) \setminus \{v\}$ as $H \subset V(K_{1,p})$, and thus $m = 0$. Therefore, (i) and (ii) hold directly from the characteristic polynomial $\mathcal{P}_Q(z)$. For $k = 1$, by $4^{(k-1)} = 4^{(0)}$, we mean 4 is not an eigenvalue. From the characteristic polynomial $\mathcal{P}_Q$, we have $4^{(k-1)}$, and $1^{(p-k-1)}$ belongs to $Spec(K_{1,p}^H)$, when $m \in \{0, 1\}$ and $1 \leq k \leq p$. Thus, (iii) holds.

(iv) Suppose $K_{1,p}^H = K_{1,p}^{m,k}$ is Q-integral. Consider the following cases according to the values of k.

Case A: $k = 0$.

We have $\mathcal{P}_Q(z) = (z-1)^{p-1}f(z)$, where $f(z) = z^2-(p+4)z+3$. Now, $f(0) = 3 > 0$ and $f(1) = -p < 0$, and so $f(z)$ has a root in $(0, 1)$. Thus, $K_{1,p}^{1,0}$ is not Q-integral.

Case B: $1 \leq k < p$.

For $m = 1$, we have $\mathcal{P}_Q(z) = (z-4)^{k-1}(z-1)^{p-k-1}f(z)$, where $f(z) = z^3 - (p + 8)z^2 + (4p + 19)z - (3k + 12)$. Here $f(z)$ has a root in $(0, 1)$.

For $m = 0$, we have $\mathcal{P}_Q(z) = (z-4)^{k-1}(z-1)^{p-k-1}g(z)$, where $g(z) = z^3 - (p + 5)z^2 + (4p + 4)z - 3k$. Note that $g(z)$ also has a root in $(0, 1)$. Hence, $K_{1,p}^{m,k}$ is not Q-integral for $1 \leq k < p$.

Case C: $k = p$.

We have $\mathcal{P}_Q(z) = (z-4)^{p-1}f(z)$, where $f(z) = z^2-(p+4)z+3p$. Then $f(0) = 3p > 0$ and $f(1) = 2p-3$, which is greater than 0 for $p \geq 2$, and less than 0 for $p = 1$. We have, $f(2) = p-4$, which is greater than 0 for $p \geq 5$, and less than 0 for $p \leq 3$. Also, $f(3) = -3 < 0$. Thus, $f(z)$ has a root in $(0,1)$ for $p = 1$, in the interval $(1,2)$ for $p = 2,3$, and in $(2,3)$ for $p \geq 5$. Thus, $Q(K_{1,p}^H) = Q(K_{1,p}^{0,p})$ has a non-integral eigenvalue for $p \neq 4$. For $p = 4$, $K_{1,4}^{0,4}$ is Q-integral with Q-eigenvalues $2,4,4,4,6$.

Hence, $K_{1,p}^H$ is Q-integral if and only if $K_{1,p}^H = K_{1,4}^{0,4}$. □

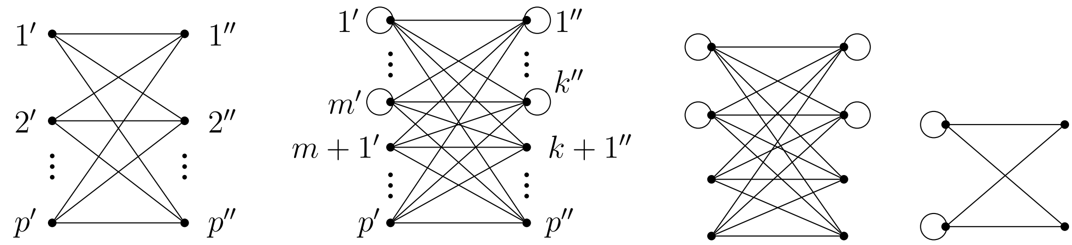
Here, we give a corollary which is a consequence of Theorem 4.3.

Corollary 4.4. *Let M be a square matrix of order $p+1$ such that $M = P^{-1}\begin{pmatrix} p & J \\ J & I_p \end{pmatrix}P$ for some permutation matrix P, and $D'_{p+1}(\neq O, I)$ be a $(0,1)$-diagonal matrix. Then $Spec(M+3D') \subseteq \mathbb{Z}$ if and only if $p = 4$ and $D' = P^{-1}\begin{pmatrix} 0 & O \\ O & I_4 \end{pmatrix}P$.*

Proof. Note that $PD'P^{-1}$ is a non-zero and non-identity $(0,1)$-diagonal matrix. We have $P(M+3D')P^{-1} = PMP^{-1} + 3PD'P^{-1} = \begin{pmatrix} p & \mathrm{J} \\ \mathrm{J} & I_p \end{pmatrix} + 3PD'P^{-1} = Q(K_{1,p}^H)$, where $\emptyset \neq H \subset V(K_{1,p})$. From Theorem 4.3(iv), we have $K_{1,p}^{m,k}$ is Q-integral if and only if $K_{1,p}^{m,k} = K_{1,4}^{0,4}$. Thus, $Spec(M+3D') \subseteq \mathbb{Z}$ if and only if $PD'P^{-1} = \begin{pmatrix} 0 & \mathrm{O} \\ \mathrm{O} & I_4 \end{pmatrix}$. Hence, the result holds. □

4.2 Complete Equipartite Graph

In this section, we discuss the Q-integrality of complete bipartite graph $K_{p,p}$ containing self-loops. Let $V(K_{p,p}) = V_1 \cup V_2$, where $V_1 = \{1', \ldots, p'\}$, $V_2 = \{1'', \ldots, p''\}$,



(a) $K_{p,p}$ (b) $K_{p,p}^{m,k}$ (c) $K_{4,4}^{2,2}$ (d) $K_{2,2}^{2,0}$

FIGURE 4.3: Complete equipartite graph $K_{p,p}$ and $K_{p,p}^{m,k}$.

and $V_1 \cap V_2 = \emptyset$. Note that $Spec(K_{p,p}) = \{0, p^{(2p-2)}, 2p\}$. Also, $Q(K_{p,p})$ is dominated by $Q(K_{p,p}^{m,k})$, and $Q(K_{p,p}^{m,k})$ is dominated by the matrix $Q(K_{p,p}^{p,p})$. Thus, we have $2p = q(K_{p,p}) \leq q(K_{p,p}^{m,k}) \leq q(K_{p,p}^{p,p}) = 2p+3$.

Here, we give a necessary and sufficient condition to have integral Q-eigenvalues of $K_{p,p}^{H}$, which is the main result of this chapter.

Theorem 4.5. *Let $\emptyset \neq H \subset V(K_{p,p})$. Then $K_{p,p}^{H}$ is Q-integral if and only if $K_{p,p}^{H} \in \{K_{4,4}^{2,2}, K_{2,2}^{2,0}\}$.*

If $H = \{1', \ldots, m', 1'', \ldots, k''\}$ where $1 \leq m, k \leq p$, then the signless Laplacian of $K_{p,p}^{H}$ corresponding to the vertex set $V(K_{p,p}^{H}) = \{1', \ldots, m', (m+1)', \ldots, p', 1'', \ldots, k''$, $(k+1)'', \ldots, p''\}$ is given by

$$Q(K_{p,p}^{H}) = \begin{pmatrix} (p+3)I_m & O & J & J \\ O & pI_{p-m} & J & J \\ J & J & (p+3)I_k & O \\ J & J & O & pI_{p-k} \end{pmatrix}. \tag{4.1}$$

If $m = 0$ (resp. $k = 0$), then $H = \{1'', \ldots, k''\}$ (resp. $H = \{1', \ldots, m'\}$), and in (4.1), the block I_0 becomes empty, that is, the rows and columns corresponding to the block I_0 do not exist. We use the matrix given in (4.1) to find the equitable quotient matrix of $Q(K_{p,p}^{H})$ for different H, that is, for different values of m, k, where $0 \leq m, k \leq p$.

Next, we prove some lemmas which are essential for proving Theorem 4.5.

Lemma 4.6. *Let* $1 \leq m \leq p$. *Then the graph* $K_{p,p}^{m,0}$ *is* Q*-integral if and only if* $m = p = 2$.

Proof. Consider the following two cases.

Case A: $m < p$.

Without any loss of generality, suppose $H = \{1', \ldots, m'\}$ where $1 \leq m < p$. Clearly, $p \geq 2$. The signless Laplacian of $K_{p,p}^{m,0}$ given in (4.1) now becomes

$$Q(K_{p,p}^{m,0}) = \begin{pmatrix} (p+3)I_m & \mathrm{O} & \mathrm{J} \\ \mathrm{O} & pI_{p-m} & \mathrm{J} \\ \mathrm{J} & \mathrm{J} & pI_p \end{pmatrix}.$$

The equitable quotient matrix $\mathcal{E}$ of $Q(K_{p,p}^{m,0})$ in (4.1) is $\begin{pmatrix} p+3 & 0 & p \\ 0 & p & p \\ m & p-m & p \end{pmatrix}$,

and the characteristic polynomial of $\mathcal{E}$ is $\mathcal{P}_{\mathcal{E}}(z) = z^3 - (3p+3)z^2 + (2p^2+6p)z - 3mp$. Now,

$$\begin{aligned}
\mathcal{P}_{\mathcal{E}}(2p) &= -\,3mp < 0, \\
\mathcal{P}_{\mathcal{E}}(2p+1) &= p(2p-3m-3) - 2 \begin{cases} > 0 & \text{if} \quad 1 \leq m < \frac{2p}{3} - 1 \\ < 0 & \text{if} \quad \frac{2p}{3} - 1 \leq m < p \end{cases}, \\
\text{and} \quad \mathcal{P}_{\mathcal{E}}(2p+2) &= 3p(p-m) + p^2 - 4 > 0.
\end{aligned}$$

Thus, $\mathcal{E}$ has a non-integral eigenvalue in $(2p, 2p+1)$ if $1 \leq m < \frac{2p}{3} - 1$, otherwise it has a non-integral eigenvalue in $(2p+1, 2p+2)$. Since $Spec(\mathcal{E}) \subseteq Spec(Q(K_{p,p}^{m,0}))$, $K_{p,p}^{m,0}$ is not Q-integral.

Case B: $m = p$.

The equitable quotient matrix of $Q(K_{p,p}^{p,0})$ in (4.1) is $\mathcal{E} = \begin{pmatrix} p+3 & p \\ p & p \end{pmatrix}$, and the characteristic polynomial of $\mathcal{E}$ is $\mathcal{P}_{\mathcal{E}}(z) = z^2 - (2p+3)z + 3p$. Observe that $\mathcal{P}_{\mathcal{E}}(z)$ has a root in $(0, 1)$ for $p = 1$, and in the interval $(1, 2)$ for $p \geq 3$. By Theorem 1.5, $Spec(\mathcal{E}) \subseteq Spec(Q(K_{p,p}^{p,0}))$, and thus $K_{p,p}^{p,0}$ is not Q-integral for $p \neq 2$. For $p = 2$, $K_{2,2}^{2,0}$ is Q-integral with Q-eigenvalues $1, 2, 5, 6$.

Hence, $K_{p,p}^{p,0}$ is Q-integral if and only if $K_{p,p}^{p,0} = K_{2,2}^{2,0}$. $\square$

Lemma 4.7. *For $1 \leq m < p$, the graph $K_{p,p}^{m,m}$ is Q-integral if and only if $K_{p,p}^{m,m} = K_{4,4}^{2,2}$.*

Proof. Let $H \subset V(G)$ be such that $K_{p,p}^{H} = K_{p,p}^{m,m}$ for $1 \leq m < p$. Without any loss of generality, suppose $H = \{1', \ldots, m', 1'', \ldots, m''\}$. The signless Laplacian $Q(K_{p,p}^{m,m})$ corresponding to the vertex set $\{1', \ldots, m', m+1', \ldots, p', 1'', \ldots, m'', m+1'', \ldots, p''\}$ is given in (4.1). The equitable quotient matrix of $Q(K_{p,p}^{m,m})$ is given by the following matrix

$$\mathcal{E} = \begin{pmatrix} p+3 & 0 & m & p-m \\ 0 & p & m & p-m \\ m & p-m & p+3 & 0 \\ m & p-m & 0 & p \end{pmatrix},$$

and the characteristic polynomial of $\mathcal{E}$ is

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(z) = z^4 - (4p+6)z^3 + (5p^2+18p+9)z^2 - (18p+6mp+12p^2+2p^3)z \\ - (9m^2 - 6mp^2 - 18mp).\end{aligned} \tag{4.2}$$

We have $\mathcal{P}_{\mathcal{E}}(0) = 9m(2p-m) + 6mp^2 > 0$. Now, consider the following two cases.

Case A: $1 \leq m < \frac{p}{3}$.

Here, $\mathcal{P}_{\mathcal{E}}(1) = -2p^2(p-3m) - p(7p-12m) - 4(p-1) - 9m^2 < 0$. Therefore, $\mathcal{P}_{\mathcal{E}}(z)$ has a solution in $(0,1)$, and thus $\mathcal{E}$ and $Q(K_{p,p}^{m,m})$ have an eigenvalue in $(0,1)$, by Theorem 1.5. Hence $K_{p,p}^{m,m}$ is not Q-integral.

Case B: $\frac{p}{3} \leq m < p$.

When $p=2$, we have $m=1$, and $\mathcal{P}_{\mathcal{E}}(2p) = \mathcal{P}_{\mathcal{E}}(4) = 3 > 0$, $\mathcal{P}_{\mathcal{E}}(2p+1) = \mathcal{P}_{\mathcal{E}}(5) = -9 < 0$. Thus $\mathcal{P}_{\mathcal{E}}(z)$ has a solution in $(4,5)$, implying that $K_{2,2}^{1,1}$ is not Q-integral. When $p \geq 3$, let $3m = p + r$, for some non-negative integer r $(0 \leq r \leq 2p-3)$. Now,

$$\begin{aligned} \mathcal{P}_{\mathcal{E}}(2p+1) &= 2p^3 - 7p^2 + 4p - 6mp^2 + 12mp - 9m^2 + 4 \\ &= -4p(p-1) - 2pr(p-1) - (r^2-4) < 0, \\ \mathcal{P}_{\mathcal{E}}(2p+2) &= 4p^3 - 4p^2 - 4p - 6mp^2 + 6mp - 9m^2 + 4, \\ \text{and} \quad \mathcal{P}_{\mathcal{E}}(2p+3) &= 6p^2(p-m) + 9(p^2-m^2) > 0. \end{aligned} \tag{4.3}$$

Then, for all values of p and r, $\mathcal{P}_{\mathcal{E}}(z)$ has a root in the intervals as given below.

- $(2p+1, 2p+2)$ if $0 \leq r < p-2$.
- $(2p+2, 2p+3)$ if $r > p-2$.

- $(0, 1)$ if $p = 3$ and $r = p - 2$.
- $(1, 2)$ if $p \geq 5$ and $r = p - 2$.

Thus, except for $p = 4, r = 2$, $\mathcal{E}$ has a non-integral eigenvalue, and hence $K_{p,p}^{m,m}$ is not Q-integral. For $p = 4$ and $r = 2$, $K_{4,4}^{m,m} = K_{4,4}^{2,2}$ is a Q-integral graph with Q-eigenvalues $1, 4, 4, 5, 6, 7, 7, 10$.

Hence, $K_{p,p}^{m,m}$ is Q-integral if and only if $K_{p,p}^{m,m} = K_{4,4}^{2,2}$. □

Lemma 4.8. *The graph $K_{p,p}^{m,k}$ is not Q-integral for $1 \leq k < m \leq p$.*

Proof. Let $H \subseteq V(G)$ be such that $K_{p,p}^{H} = K_{p,p}^{m,k}$ for $1 \leq m \leq p$. Without any loss of generality, suppose $H = \{1', \ldots, m', 1'', \ldots, k''\}$. Depending on m, we discuss the proof in two cases.

Case A: $m = p$.

The equitable quotient matrix $\mathcal{E}$ of $Q(K_{p,p}^{m,k})$ in (4.1) is given by

$$\mathcal{E} = \begin{pmatrix} p+3 & k & p-k \\ p & p+3 & 0 \\ p & 0 & p \end{pmatrix}.$$

The characteristic polynomial of $\mathcal{E}$ is

$$\mathcal{P}_{\mathcal{E}}(z) = z^3 - (3p+6)z^2 + (2p^2 + 12p + 9)z - (9p + 3kp + 3p^2).$$

Now,

$$\mathcal{P}_{\mathcal{E}}(2p+1) = -\,p^2 - 3kp + 4 < 0,$$

$$\mathcal{P}_{\mathcal{E}}(2p+2) = p(p-3k-3)+2 \begin{cases} > 0 & \text{if } \ k \leq \frac{p}{3} - 1 \\ < 0 & \text{otherwise} \end{cases},$$

and $\mathcal{P}_{\mathcal{E}}(2p+3) = 3p(p-k) > 0.$

Therefore, $\mathcal{P}_{\mathcal{E}}(z)$ has a non-integral eigenvalue in $(2p+1, 2p+2)$ if $k \leq \frac{p}{3} - 1$, otherwise it has non-integral eigenvalue in $(2p+2, 2p+3)$. By Theorem 1.5, $Spec(\mathcal{E}) \subseteq Q(K_{p,p}^{m,k})$, and therefore $K_{p,p}^{m,k}$ is not Q-integral.

Case B: $m < p$.

Since $1 \leq k < m < p$, we have $p \geq 3$. The equitable quotient matrix $\mathcal{E}$ of the signless Laplacian $Q(K_{p,p}^{m,k})$ in (4.1) is given by

$$\mathcal{E} = \begin{pmatrix} p+3 & 0 & k & p-k \\ 0 & p & k & p-k \\ m & p-m & p+3 & 0 \\ m & p-m & 0 & p \end{pmatrix}.$$

The characteristic polynomial of $\mathcal{E}$ is

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(z) = z^4 - (4p+6)z^3 + (5p^2+18p+9)z^2 - (18p+3kp+3mp+12p^2+2p^3)z \\ + (9kp - 9km + 9mp + 3kp^2 + 3mp^2).\end{aligned}$$

Now,

$$\begin{aligned}
\mathcal{P}_{\mathcal{E}}(2p) &= -3kp(p-3) - 3mp(p-3) - 9km < 0,\\
\mathcal{P}_{\mathcal{E}}(2p+1) &= 2p^3 - 7p^2 + 4p + 4 - 3p(p-2)(k+m) - 9km,\\
\mathcal{P}_{\mathcal{E}}(2p+2) &= 4p^3 - 4p^2 - 4p - 3kp^2 - 3mp^2 - 9km + 3kp + 3mp + 4,\\
\text{and}\ \ \mathcal{P}_{\mathcal{E}}(2p+3) &= 3p^2(p-k) + 3p^2(p-m) + 9(p^2 - km) > 0.
\end{aligned} \tag{4.4}$$

Since $p, m \in \mathbb{N}$ and $p > m$, let $p = m + l$, for some $l \in \mathbb{N}$.

Note that $p \geq k + l + 1$. Putting $m = p - l$ in equation (4.4), we get

$$\begin{aligned}
\mathcal{P}_{\mathcal{E}}(2p+1) &= 2p^3 - 7p^2 + 4p + 4 - 3p(p-2)(p+k-l) - 9k(p-l),\\
\mathcal{P}_{\mathcal{E}}(2p+2) &= 4p^3 - 4p^2 - 4p - 3p(p-1)(p+k-l) - 9k(p-l) + 4.
\end{aligned} \tag{4.5}$$

In order to prove the lemma, we observe from Theorem 1.5 and equation (4.4), that it is sufficient to show $\mathcal{P}_{\mathcal{E}}(z) \neq 0$ for $x = 2p+1, 2p+2$. We start by proving $\mathcal{P}_{\mathcal{E}}(2p+1) \neq 0$.

Claim 1: $\mathcal{P}_{\mathcal{E}}(2p+1) \neq 0$.

We prove Claim 1 using Claims 1.1 and 1.2.

Claim 1.1: $\mathcal{P}_{\mathcal{E}}(2p+1) < 0$ for $1 \leq l \leq 2k+2$.

We use mathematical induction on k to prove this claim. For $k = 1$, we have $1 \leq l \leq 4$, and from equation (4.5), we have $\mathcal{P}_{\mathcal{E}}(2p+1) < 0$ as $p \geq l + k + 1$. Thus, the claim is true for $k = 1$. Suppose the claim is true for $k = k_1$, which implies,

$$\begin{aligned}
\mathcal{P}_{\mathcal{E}}(2p+1) &= 2p^3 - 7p^2 + 4p + 4 - 3p(p-2)(p+k_1-l) - 9k_1(p-l)\\
&< 0, \ \text{for}\ 1 \leq l \leq 2k_1 + 2.
\end{aligned} \tag{4.6}$$

For $k = k_1$, $l = 2k_1 + 2$, we get from above equation,

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(2p+1) &= 2p^3 - 7p^2 + 4p + 4 - 3p(p-2)(p-k_1-2) - 9k_1(p-2k_1-2) \\ &< 0.\end{aligned} \tag{4.7}$$

We prove that Claim 1.1 is also true for $k = k_1 + 1$, that is,

$$\mathcal{P}_{\mathcal{E}}(2p+1) < 0, \quad \text{for} \ \ 1 \leq l \leq 2k_1 + 4.$$

Note that $p - l = m \geq 2$. At $k = k_1 + 1$, we have the following from equation (4.5).

- $1 \leq l \leq 2k_1 + 2$:

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(2p+1) &= 2p^3 - 7p^2 + 4p + 4 - 3p(p-2)(p+k_1+1-l) - 9(k_1+1)(p-l) \\ &\leq 2p^3 - 7p^2 + 4p + 4 - 3p(p-2)(p+k_1-l) - 9k_1(p-l) \\ &< 0, \qquad \text{[using equation (4.6)]}.\end{aligned}$$

- $l = 2k_1 + 3$:

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(2p+1) = 2p^3 - 7p^2 + 4p + 4 - 3p(p-2)(p-k_1-2) - 9k_1(p-2k_1-2) - \\ 9(p-3k_1-3) < 0, \ \text{[using equation (4.7) and } p - 2k_1 - 3 > 0].\end{aligned}$$

- $l = 2k_1 + 4$:

  In this case, $p \geq 3k_1 + 6$, and we have

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(2p+1) &= -9k_1^2 - 33k_1 - 26 < 0, \quad \text{when} \ \ p = 3k_1 + 6, \\ \mathcal{P}_{\mathcal{E}}(2p+1) &= -18k_1^2 - 78k_1 - 72 < 0, \quad \text{when} \ \ p = 3k_1 + 7, \\ \text{and} \ \ \mathcal{P}_{\mathcal{E}}(2p+1) &\leq -27k_1^2 - 135k_1 - 144 < 0, \quad \text{when} \ \ p \geq 3k_1 + 8.\end{aligned}$$

  Therefore, $\mathcal{P}_{\mathcal{E}}(2p+1) < 0$ for $k = k_1 + 1$, $l = 2k_1 + 4$.

Thus, Claim 1.1 is true for $k = k_1 + 1$. Hence, we conclude that Claim 1.1 is true.

Since $p \geq k + l + 1$, let $p = k + l + s$, for some $s \in \mathbb{N}$.

Claim 1.2: If $l \geq 2k + 3$, then

$$\mathcal{P}_{\mathcal{E}}(2p+1) \begin{cases} > 0 & \text{if } 1 \leq s \leq 2l - 4k - 4 \\ < 0 & \text{otherwise.} \end{cases}$$

Since $l \geq 2k + 3$, let $l = 2k + 3 + r$, for some $r \in \mathbb{N} \cup \{0\}$. Putting $p = k + l + s = 3k + r + s + 3$ in equation (4.5), we get

$$\begin{aligned} \mathcal{P}_{\mathcal{E}}(2p+1) = {} & 2r^3 + 18k^2r + 12kr^2 + 18k^2 + 11r^2 + 42kr + 30k + 16r + 7 \\ & + 7s + 3r^2s + 6krs + 10rs - 9k^2s - 6ks^2 - 3ks - s^3 - s^2. \end{aligned} \tag{4.8}$$

To prove Claim 1.2, consider the following cases.

Case 1.2.1 $1 \leq s \leq 2l - 4k - 4$.

In this case, $1 \leq s \leq 2r + 2$ as $l = 2k + 3 + r$, and thus, from equation (4.8), we get

$$\begin{aligned} \mathcal{P}_{\mathcal{E}}(2p+1) &= (2r^3 + 3sr^2 + 10rs + 7 + 6r - s^3) + (6krs + 12kr^2 + 36kr + 26k - 6ks^2) \\ &\quad + (11r^2 + 7s - s^2) + (18k^2r + 18k^2 - 9k^2s) + (6kr + 4k - 3ks + 10r) \\ &\geq 9r^2 + 16r + s + 7 > 0. \end{aligned}$$

Case 1.2.2 $s > 2l - 4k - 4$.

We have $s > 2l - 4k - 4 = 2r + 2$, i.e., $s = 2r + 2 + t$, for some $t \in \mathbb{N}$. Thus, equation (4.8), becomes

$$\mathcal{P}_{\mathcal{E}}(2p+1) = -9r^2(t-1) - 18r(t-1) - 9(t-1) - 18krt - t^3 - 6rt^2 - 6kt^2$$
$$- 27kt - 7t^2 - 9k^2t < 0.$$

From Cases 1.2.1-1.2.2, we conclude that Claim 1.2 holds true.

Therefore, from Claims 1.1-1.2, we get $\mathcal{P}_{\mathcal{E}}(2p+1) \neq 0$.

Next, we prove that $2p+2$ is also not a root of $\mathcal{P}_{\mathcal{E}}(x)$ through the following claim. Recall that $p = k + l + s$, for some $s \in \mathbb{N}$.

Claim 2:

$$\mathcal{P}_{\mathcal{E}}(2p+2) \begin{cases} < 0 & \text{if } 1 \leq s \leq 2k - 4l + 3 \\ > 0 & \text{otherwise.} \end{cases}$$

We prove the claim by making three cases as follows.

Case 2.1 $1 \leq s \leq 2k - 4l + 3$.

Here, $2k - 4l + 3 > 0$, i.e., $l < \frac{k}{2} + 1$, i.e., $l \leq \lfloor \frac{k}{2} \rfloor + 1$, i.e., $l = \lfloor \frac{k}{2} \rfloor + 1 - r$, for some non-negative integer $r (0 \leq r \leq \lfloor \frac{k}{2} \rfloor)$. Note that $r \geq 1$ when k is even.

Case 2.1.1 k is an even number, that is, $k = 2k_1$, $k_1 \in \mathbb{N}$.

We have $l = \lfloor \frac{k}{2} \rfloor + 1 - r = k_1 + 1 - r$, and $p = k + l + s = 3k_1 + s + 1 - r$. Putting these values of p, k, l in equation (4.5), we get

$$\mathcal{P}_{\mathcal{E}}(2p+2) = s^3 + 5s^2 + 9k_1^2 s + 6k_1 s^2 + 9k_1 s + 8r^2 + 24k_1 r^2 + 9sr^2 - 6s^2 r - 30k_1 sr$$
$$- 36k_1 r - 13sr - 4r^3 - 36k_1^2 r.$$

We have $1 \le s \le 2k - 4l + 3$, i.e., $1 \le s < 4r$, where $1 \le r \le k_1$. To prove Claim 2, it is sufficient to show that

$$\mathcal{P}_{\mathcal{E}}(2p+2) < 0, \quad \text{for } 1 \le s < 4r \text{ where } 1 \le r \le k_1. \tag{4.9}$$

We prove the above statement using induction on k_1. When $k_1 = 1$, we have $r = 1$, and $1 \le s \le 3$, and thus $\mathcal{P}_{\mathcal{E}}(2p+2) = s^3 - 5s^2 - 16s - 44 < 0$. Suppose (4.9) is true for $k_1 = k_1'$, that is,

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(2p+2) = {} & s^3 + 5s^2 + 9k_1'^2 s + 6k_1' s^2 + 9k_1' s + 8r^2 + 24k_1' r^2 + 9sr^2 \\ & - 6s^2 r - 30k_1' sr - 36k_1' r - 13sr - 4r^3 - 36k_1'^2 r \\ < {} & 0, \quad \text{for } 1 \le s < 4r \text{ where } 1 \le r \le k_1'.\end{aligned} \tag{4.10}$$

At $k_1 = k_1' + 1$, we get $\mathcal{P}_{\mathcal{E}}(2p+2) = \phi_1 + \phi_2$,

$$\begin{aligned}\text{where } \phi_1 = {} & s^3 + 5s^2 + 9k_1'^2 s + 6k_1' s^2 + 9k_1' s + 8r^2 + 24k_1' r^2 + 9sr^2 - 6s^2 r - 30k_1' sr \\ & - 36k_1' r - 13sr - 4r^3 - 36k_1'^2 r, \\ \text{and } \phi_2 = {} & 18k_1' s + 18s + 6s^2 + 24r^2 - 30sr - 72r - 72k_1' r.\end{aligned}$$

We need to prove that $\mathcal{P}_{\mathcal{E}}(2p+2) < 0$, for $1 \le s < 4r$ where $1 \le r \le k_1' + 1$. Consider $1 \le r \le k_1'$. Since $1 \le s < 4r$, we get $\phi_1 < 0$ by equation (4.10), and

$$\begin{aligned}\phi_2 &= 6[3s(k_1' - r) + s(s - 2r) + 3s + 4r^2 - 12r - 12k_1' r] \\ &\le -6[2r(4r - s) + 2(4r - s) + 3k_1' + r] < 0.\end{aligned}$$

At $r = k_1' + 1$, we have $1 \leq s < 4r$, i.e., $1 \leq s \leq 4k_1' + 3$, and therefore

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(2p+2) &= s^3 + 5s(s-1) - 11s - 12k_1'^2 s - 28k_1' s - 76k_1'^2 - 104k_1' - 16k_1'^3 - 44 \\ &\leq s^3 + 4s - 8k_1' s - 124k_1' - 12k_1'^2 s - 76k_1'^2 - 16k_1'^3 - 59 \\ &\leq -4k_1'^2(4k_1' + 3 - s) - 4k_1'(4k_1' + 3 - s) - 12k_1'(4k_1' + 3 - s) \\ &\quad - 13(4k_1' + 3 - s) - 24k_1' - 20 < 0.\end{aligned}$$

So, we conclude that (4.9) is true for $k_1 = k_1' + 1$, and thus true for every $k_1 \in \mathbb{N}$. Hence, if k is even, then $P_{\mathcal{E}}(2p + 2) < 0$ for $1 \leq s \leq 2k - 4l + 3$.

Case 2.1.2 k is an odd number, that is, $k = 2k_1 + 1$, $k_1 \in \mathbb{N} \cup \{0\}$.

In this case, $l = k_1 + 1 - r$, and $p = 3k_1 + s + 2 - r$. From equation (4.5), we get

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(2p+2) &= -18k_1^2 - 30k_1 - 36k_1^2 r - 30k_1 sr - 6s^2 r - 19sr - 5s - 9 - 4r^3 - 10r \\ &\quad - 48k_1 r + 14r^2 + 24k_1 r^2 + 9sr^2 + 9k_1^2 s + 6k_1 s^2 + 3k_1 s + s^3 + 5s^2.\end{aligned}$$

We have $1 \leq s \leq 2k - 4l + 3$, i.e., $1 \leq s \leq 4r + 1$, where $0 \leq r \leq k_1$. To prove the claim, it is sufficient to show that

$$\mathcal{P}_{\mathcal{E}}(2p+2) < 0, \quad \text{for } \ 1 \leq s \leq 4r + 1 \ \text{ where } \ 0 \leq r \leq k_1. \tag{4.11}$$

We use induction on k_1. For $k_1 = 0$, we have $\mathcal{P}_{\mathcal{E}}(2p + 2) = -8 < 0$. For $k_1 = 1$, we have $r = 0, 1$. Here,

$$\begin{aligned}\mathcal{P}_{\mathcal{E}}(2p+2) &= \begin{cases} -38, & \text{if } r = 0 \text{ and } s = 1 \\ (s^3 - 25s) + (5s^2 - 8s - 117), & \text{if } r = 1 \text{ and } 1 \leq s \leq 5 \end{cases} \\ &< 0.\end{aligned}$$

Let (4.11) be true for $k_1 = k_1'$, that is,

$$\mathcal{P}_{\mathcal{E}}(2p+2) < 0, \quad \text{for } \ 1 \leq s \leq 4r+1 \ \text{ where } \ 0 \leq r \leq k_1'. \tag{4.12}$$

Let $k_1 = k_1' + 1$. Then we have $\mathcal{P}_{\mathcal{E}}(2p+2) = \phi_1 + \phi_2$, where

$$\begin{aligned}
\phi_1 &= -18k_1'^2 - 30k_1' - 36k_1'^2 r - 30k_1' sr - 6s^2 r - 19sr - 5s - 9 - 4r^3 - 10r \\
&\quad - 48k_1' r + 14r^2 + 24k_1' r^2 + 9sr^2 + 9k_1'^2 s + 6k_1' s^2 + 3k_1' s + s^3 + 5s^2, \\
\text{and } \ \phi_2 &= -36k_1' - 72k_1' r - 84r - 30sr - 48 + 24r^2 + 18k_1' s + 12s + 6s^2.
\end{aligned}$$

For $0 \leq r \leq k_1'$, we have $1 \leq s \leq 4r+1$, and $\phi_1 < 0$ using equation (4.12), and

- if $1 \leq s \leq 4r-1$, then

$$\begin{aligned}
\phi_2 &= 18s(k_1' - r) - 12sr - 36k_1' - 72k_1' r - 84r - 48 + 24r^2 + 12s + 6s^2 \\
&\leq -54r - 54k_1' - 54 < 0.
\end{aligned}$$

- if $s = 4r$, then $\phi_2 = -36k_1' - 36r - 48 < 0$
- if $s = 4r+1$, then $\phi_2 = -18k_1' - 18r - 30 < 0$.

When $r = k_1' + 1$, we get for $1 \leq s \leq 4r+1$,

$$\begin{aligned}
\mathcal{P}_{\mathcal{E}}(2p+2) &= s^3 + 5s^2 - 100k_1'^2 - 192k_1' - 117 - 16k_1'^3 - 12k_1'^2 s - 40k_1' s - 33s \\
&\leq 4k_1'^2 s + 20k_1' s + 17s - 16k_1'^3 - 100k_1'^2 - 192k_1' - 117 \\
&\leq -24k_1' - 32 < 0.
\end{aligned}$$

Hence, $\mathcal{P}_{\mathcal{E}}(2p+2) < 0$ for $1 \leq s \leq 4r+1$ where $0 \leq r \leq k_1'+1$. Thus, (4.11) is true for all $k_1 \in \mathbb{N} \cup \{0\}$. Therefore, if k is odd, then $\mathcal{P}_{\mathcal{E}}(2p+2) < 0$ for $1 \leq s \leq 2k-4l+3$.

From Cases 2.1.1-2.1.2, we conclude that $\mathcal{P}_{\mathcal{E}}(2p+2) < 0$ for $1 \leq s \leq 2k-4l+3$.

Case 2.2 $s \geq 2k - 4l + 4 \geq 1$.

In this case, $2k - 4l + 4 > 0$, i.e., $l < \frac{k}{2} + 1$, i.e., $l = \lfloor \frac{k}{2} \rfloor + 1 - r$, for some non-negative integer $r (0 \leq r \leq \lfloor \frac{k}{2} \rfloor)$. Note that $r \geq 1$ when k is even. Now, $s \geq 2k - 4l + 4 = 2k - 4\lfloor \frac{k}{2} \rfloor + 4r$, i.e., $s = 2k - 4\lfloor \frac{k}{2} \rfloor + 4r + t$, for some $t \in \mathbb{N} \cup \{0\}$. Thus from equation (4.5), we get

$$\mathcal{P}_{\mathcal{E}}(2p+2) = \begin{cases} t^3 + 36r^2 + 5t^2 + 9r^2t + 6rt^2 + 9k_1^2t + 6k_1t^2 + \\ 18k_1rt + 40rt, & \text{if } k = 2k_1,\ k_1 \in \mathbb{N} \\ \\ t^3 + 9k_1^2t + 6k_1t^2 + 9r^2t + 6rt^2 + 36r^2 + & \text{if } k = 2k_1 + 1, \\ 18k_1rt + 11t^2 + 36r + 45rt + 27k_1t + 27t + 9, & k_1 \in \mathbb{N} \cup \{0\} \end{cases}$$
$$> 0.$$

Case 2.3 $s \geq 1 > 2k - 4l + 4$.

In this case, $2k - 4l + 4 \leq 0$, i.e., $l \geq \frac{k}{2} + 1$, i.e., $l = \lceil \frac{k}{2} \rceil + 1 + r$, for some non-negative integer r. Putting $p = k + l + s$ in equation (4.5), we get

$$\mathcal{P}_{\mathcal{E}}(2p+2) = \begin{cases} s^3 + 5s^2 + 4r^3 + 8r^2 + 36k_1^2r + 24k_1r^2 + 9k_1^2s + \\ 9r^2s + 6k_1s^2 + 6s^2r + 36k_1r + 9k_1s + 13rs + & \text{if } k = 2k_1,\ k_1 \in \mathbb{N} \\ 30k_1rs, \\ \\ s^3 + 4r^3 + 26r^2 + 11s^2 + 18k_1^2 + 36k_1^2r + \\ 24k_1r^2 + 9k_1^2s + 9r^2s + 6k_1s^2 + 6s^2r + 96k_1r + & \text{if } k = 2k_1 + 1, \\ 50r + 33k_1s + 23s + 30k_1rs + 37rs + 42k_1 + 19, & k_1 \in \mathbb{N} \cup \{0\} \end{cases}$$
$$> 0.$$

From Cases 2.1-2.3, we conclude that Claim 2 holds. By Theorem 1.5, $Spec(\mathcal{E}) \subseteq Q(K_{p,p}^{m,k})$. So, $K_{p,p}^{m,k}$ has a Q-eigenvalue in at least one of the intervals $(2p, 2p+1), (2p+1, 2p+2)$, or $(2p+2, 2p+3)$. Hence, $K_{p,p}^{m,k}$ is not Q-integral in Case B.

From Cases A-B, we conclude that the lemma holds. □

Proof of Theorem 4.5. Without any loss of generality, suppose $H = H_1 \cup H_2$ such that $H_i \subseteq V_i$ for $i = 1, 2$. For the non-isomorphic choices of H, let $0 \le k \le m \le p$, where $|H_1| = m, |H_2| = k$.

- $k = 0$: By Lemma 4.6, $K_{p,p}^{m,0}$ is Q-integral if and only if $K_{p,p}^{m,0} = K_{2,2}^{2,0}$.
- $m = k$: From Lemma 4.7, we get $K_{p,p}^{m,m}$ is Q-integral if and only if $K_{p,p}^{m,m} = K_{4,4}^{2,2}$.
- $1 \le k < m \le p$: By Lemma 4.8, $K_{p,p}^{m,k}$ is not Q-integral.

Hence, $K_{p,p}^{H}$ is Q-integral if and only if $K_{p,p}^{H} \in \{K_{2,2}^{2,0}, K_{4,4}^{2,2}\}$. □

Now, we give a corollary which follows from Theorem 4.5.

Corollary 4.9. *Let M be a square matrix of order $2p$ such that $M = P^{-1}\begin{pmatrix} O_p & J \\ J & O_p \end{pmatrix} P$ for some permutation matrix P, and $D'_{2p}(\neq O, I)$ be a $(0,1)$-diagonal matrix. Then $Spec(M + 3D') \subseteq \mathbb{Z}$ if and only if either $p = 2$, $D' = P^{-1}\begin{pmatrix} I_2 & O \\ O & O_2 \end{pmatrix} P$, or $p = 4$, $D' = P^{-1}\begin{pmatrix} D''_{4\times 4} & O \\ O & D'''_{4\times 4} \end{pmatrix} P$, where D'', D''' both have exactly two 1 on the diagonals.*

Proof. Note that $PD'P^{-1}$ is a non-zero and non-identity $(0,1)$-diagonal matrix. Also, $P(pI_{2p} + M + 3D')P^{-1} = pI_{2p} + PMP^{-1} + 3PD'P^{-1} = \begin{pmatrix} pI_p & \mathrm{J} \\ \mathrm{J} & pI_p \end{pmatrix} + 3PD'P^{-1} = Q(K_{p,p}^{H})$, where $\emptyset \neq H \subset V(K_{p,p})$. From Theorem 4.5, $K_{p,p}^{H}$ is Q-integral if and only if $K_{p,p}^{H} \in \{K_{2,2}^{2,0}, K_{4,4}^{2,2}\}$. Hence, the result follows. □

4.3 Conclusion

In this chapter, we studied the Q-integrality of complete bipartite graph $K_{q,p}$ after adding self-loops in the vertices of $H \subseteq V(K_{q,p})$ when $q \in \{1, p\}$. We proved that $K_{q,p}^{H}$, for $q \in \{1, p\}$, is Q-integral if and only if $K_{q,p}^{H} \in \{K_{q,p}^{0,0}, K_{q,p}^{q,p}, K_{1,4}^{0,4}, K_{2,2}^{2,0}, K_{4,4}^{2,2}\}$. Using these results, we also answered the question of when $Spec(M + 3D') \subseteq \mathbb{Z}$, where M is permutation similar to either $\begin{pmatrix} \mathrm{O}_p & \mathrm{J} \\ \mathrm{J} & \mathrm{O}_p \end{pmatrix}$ or $\begin{pmatrix} p & \mathrm{J} \\ \mathrm{J} & I_p \end{pmatrix}$, and D' is a $(0, 1)$-diagonal matrix.

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