Energy Comparison of Unicyclic Graphs with Cycle C_3

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Abstract: **In this paper, we compare the energies of unicyilc graphs with cycle C_3 (with k number of vertices, having the unique cycle C_3 denoted by $G'_{i,k}$), using the coefficients of the characteristic polynomials and Coulson integral formula by establishing the quasi-ordering '≤' on the unicyclic graphs of same order k.**

Keywords. **Energy; Characteristic polynomial; Adjacency matrix $A(G)$; Coefficient of λ^i; Unicyclic graphs; Bipartite graphs.**

1. INTRODUCTION

Let G be a simple graph with k vertices and $A(G)$ be its adjacency matrix. Let $\lambda_1, \ldots, \lambda_k$ be the eigenvalues of $A(G)$. Then the *energy* of G, denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^{k} |\lambda_i|$.

The characteristic polynomial $\det(xI - A(G))$ of the adjacency matrix $A(G)$ of the graph G is also called the *characteristic polynomial* of G is written as

$$\phi(G,x) = \sum_{i=0}^{k} a_i(G)\ x^{k-i}.$$

Using the coefficients $a_i(G)$ of $\phi(G,x)$, the energy $E(G)$ of the graph G with k vertices can be expressed by the following Coulson integral formula (Eq. (3.11) in [2]):

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{1}{x^2}\log\left[\left(\sum_{i=0}^{\lfloor\frac{k}{2}\rfloor}(-1)^i a_{2i}(G)\,x^{2i}\right)^2+\left(\sum_{i=0}^{\lfloor\frac{k}{2}\rfloor}(-1)^i a_{2i+1}(G)\,x^{2i+1}\right)^2\right]\mathrm{d}x.$$

We write $b_i(G) = |a_i(G)|$. Then clearly $b_0(G) = 1$, $b_1(G) = 0$ and $b_2(G)$ equals the number of edges of G.

About the signs of the coefficients of the characteristic polynomials of unicyclic graphs, we have the following result:

Lemma 1.1: (Lemma 1 in [3]) Let G be a unicyclic graph and the length of the unique cycle of G be `. Then we have the following:

(1) $b_{2i}(G) = (-1)^i a_{2i}(G)$,

(2) $b_{2i+1}(G) = (-1)^i a_{2i+1}(G)$, if G contain a cycle of length l with $l \equiv 1 (\text{mod } 4)$,

(3) $b_{2i+1}(G) = (-1)^{i+1} a_{2i+1}(G)$, if G contain a cycle of length l with $l \not\equiv 1 (\text{mod } 4)$.

Thus, the Coulson integral formula for unicyclic graphs can be rewritten in terms of $b_i(G)$ as follows:

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{1}{x^2}\log\left[\left(\sum_{i=0}^{\lfloor\frac{k}{2}\rfloor} b_{2i}(G)\ x^{2i}\right)^2+\left(\sum_{i=0}^{\lfloor\frac{k}{2}\rfloor} b_{2i+1}(G)\ x^{2i+1}\right)^2\right]\mathrm{d}x.$$

Hence it follows that for unicyclic graphs G, $E(G)$ is a strictly monotonically increasing function of $b_i(G)$, $i = 0, \ldots, k$. To make it more precise, we define a quasi-order ≤ on graphs as follows:

Definition 1.2: Let G_1 and G_2 be two graphs of order k. If $b_i(G_1) \le b_i(G_2)$ for all i with $1 \le i \le k$, then we write $G_1 \le G_2$.

Thus using Coulson integral formula, we have,

Theorem 1.3: For any two unicyclic graphs G_1 and G_2 of order k, we have,

$$G_1 \le G_2 \Longrightarrow E(G_1) \le E(G_2).$$

Thus, for comparing the energies of any two unicyclic graphs of the same order, it is enough to establish the quasi-order.

Using this idea, in Section 2, we compare the energies of the *unicyclic graphs* $G'_{1,k}$, $G'_{2,k}$, $G'_{3,k}$

and $G'_{4,k}$ (see Fig. 2.1 and Fig. 2.2) with k vertices having the
unique cycle C_3 by establishing the quasi-ordering:

$$G'_{2,k} \le G'_{4,k} \le G'_{3,k} \le G'_{1,k}.$$

This would imply, by above discussion,

$$E(G'_{2,k}) \le E(G'_{4,k}) \le E(G'_{3,k}) \le E(G'_{1,k}).$$

We note that these graphs are *bipartite*. For a bipartite graph G, the characteristic polynomial is of the form

$$\phi(G,x) = \sum_{i=0}^{k} a_i \; x^{k-i} = \sum_{j=0}^{\lfloor \frac{k}{2} \rfloor} a_{2j} \; x^{k-2j},$$

as $a_{2j+1} = 0$ for $j = 1, \ldots, \left\lfloor \frac{k}{2} \right\rfloor$. Also, $(-1)^j a_{2j} = b_{2j}$ and so

$$\phi(G,x) = \sum_{j=0}^{\lfloor \frac{k}{2} \rfloor} (-1)^j b_{2j} x^{k-2j}$$

Thus, for a bipartite graph G, the Coulson integral formula
reduces to

$$E(G) \;=\; \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{x} \log\left[\left(\sum_{j=0}^{\lfloor \frac{k}{2} \rfloor} (-1)^j a_{2j}(G) \right.\right.$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{x} \log\left[\left(\sum_{j=0}^{\lfloor \frac{k}{2} \rfloor} b_{2j}(G) \; x^{k-2j}\right)^2\right] \mathrm{d}x,$$

from which the monotonicity of the $E(G)$ with respect to the $b_i(G)$, $1 \le i \le k$, follows. i.e., if G_1 and G_2 are two bipartite graphs of order k such that $b_i(G_1) \le b_i(G_2)$ for all i, $1 \le i \le k$, then $E(G_1) \le E(G_2)$. i.e., $G_1 \le G_2$ implies $E(G_1) \le E(G_2)$.

2. COMPARING THE ENERGIES OF THE GRAPHS $G'_{i,k}$

We note that in the following the binomial coefficient $\binom{a}{b}$ will be zero whenever the number a is not a positive integer or the number b is not a non-negative integer.

Theorem 2.1: Let $G'_{1,k} = (V, X)$ be the graph with k vertices given below:

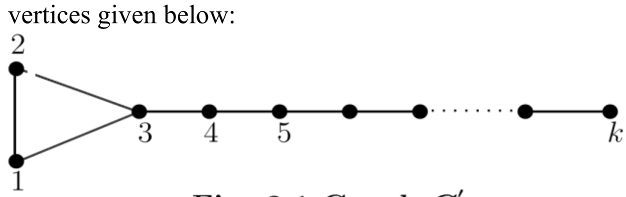

Fig. 2.1 Graph $G'_{1,k}$

Let $A(G'_{1,k}) = (a_{ij})$ be the adjacency matrix of the graph $G'_{1,k}$. Then, for $k \ge 4$, its characteristic polynomial $\chi(G'_{1,k}; \lambda)$ is given by:

$$\chi(G'_{1,k}; \lambda) = (\lambda^2 - 1) \; \chi(P_{k-2}) - 2(\lambda + 1) \; \chi(P_{k-3}) \qquad (1)$$

Also for $1 \le i \le k$, the coefficient of λ^i in $\chi(G'_{1,k}; \lambda)$ is

$$(-1)^{\frac{k-i}{2}} \left[\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}} + \binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} \right] + 2(-1)^{\frac{k-i-1}{2}} \binom{\frac{k+i-3}{2}}{\frac{k-i-3}{2}} \qquad (2)$$

In the above, when $k - i \equiv 1 (\text{mod } 2)$, the first sum vanishes and when $k \equiv i (\text{mod } 2)$, second sum vanishes.

Proof: The adjacency matrix $A(G'_{1,k})$ is given by

$$A(G'_{1,k}) = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$

The characteristic polynomial of the adjacency matrix $A(G'_{1,k})$ is given by $\chi(G'_{1,k}; \lambda) = |\lambda I - A|$, where I is the identity matrix of order k. Thus, by expanding the following determinant and the subsequent determinants by their first column, we get,

$$\chi(G'_{1,k};\lambda)=\begin{vmatrix}\lambda & -1 & -1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0\\ -1 & \lambda & -1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0\\ -1 & -1 & \lambda & -1 & 0 & 0 & 0 & \cdots & 0 & 0\\ 0 & 0 & -1 & \lambda & -1 & 0 & 0 & \cdots & 0 & 0\\ 0 & 0 & 0 & -1 & \lambda & -1 & 0 & \cdots & 0 & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & -1 & \lambda\end{vmatrix}_k$$

$$=\lambda\begin{vmatrix}\lambda & -1 & 0 & \cdots & 0\\ -1 & \lambda & -1 & \cdots & 0\\ 0 & -1 & \lambda & \cdots & 0\\ 0 & 0 & -1 & \cdots & 0\\ \vdots & \vdots & \vdots & \cdots & \vdots\\ 0 & 0 & 0 & \cdots & \lambda\end{vmatrix}_{k-1}+\begin{vmatrix}-1 & -1 & 0 & \cdots & 0\\ -1 & \lambda & -1 & \cdots & 0\\ 0 & -1 & \lambda & \cdots & 0\\ 0 & 0 & -1 & \cdots & 0\\ \vdots & \vdots & \vdots & \cdots & \vdots\\ 0 & 0 & 0 & \cdots & \lambda\end{vmatrix}_{k-1}-\begin{vmatrix}-1 & -1 & 0 & \cdots & 0\\ \lambda & -1 & 0 & \cdots & 0\\ 0 & -1 & \lambda & \cdots & 0\\ 0 & 0 & -1 & \cdots & 0\\ \vdots & \vdots & \vdots & \cdots & \vdots\\ 0 & 0 & 0 & \cdots & \lambda\end{vmatrix}_{k-1}$$

$$=\lambda^2\begin{vmatrix}\lambda & -1 & 0 & \ldots & 0\\ -1 & \lambda & -1 & \ldots & 0\\ 0 & -1 & \lambda & \ldots & 0\\ 0 & 0 & -1 & \ldots & 0\\ \vdots & \vdots & \vdots & \ldots & \vdots\\ 0 & 0 & 0 & \ldots & \lambda\end{vmatrix}_{k-2}+\lambda\begin{vmatrix}-1 & 0 & 0 & \ldots & 0\\ -1 & \lambda & -1 & \ldots & 0\\ 0 & -1 & \lambda & \ldots & 0\\ 0 & 0 & -1 & \ldots & 0\\ \vdots & \vdots & \vdots & \ldots & \vdots\\ 0 & 0 & 0 & \ldots & \lambda\end{vmatrix}_{k-2}-\begin{vmatrix}\lambda & -1 & 0 & \ldots & 0\\ -1 & \lambda & -1 & \ldots & 0\\ 0 & -1 & \lambda & \ldots & 0\\ 0 & 0 & -1 & \ldots & 0\\ \vdots & \vdots & \vdots & \ldots & \vdots\\ 0 & 0 & 0 & \ldots & \lambda\end{vmatrix}_{k-2}$$

$$+\begin{vmatrix}-1 & 0 & 0 & \ldots & 0\\ -1 & \lambda & -1 & \ldots & 0\\ 0 & -1 & \lambda & \ldots & 0\\ 0 & 0 & -1 & \ldots & 0\\ \vdots & \vdots & \vdots & \ldots & \vdots\\ 0 & 0 & 0 & \ldots & \lambda\end{vmatrix}_{k-2}+\begin{vmatrix}-1 & 0 & 0 & \ldots & 0\\ -1 & \lambda & -1 & \ldots & 0\\ 0 & -1 & \lambda & \ldots & 0\\ 0 & 0 & -1 & \ldots & 0\\ \vdots & \vdots & \vdots & \ldots & \vdots\\ 0 & 0 & 0 & \ldots & \lambda\end{vmatrix}_{k-2}+\lambda\begin{vmatrix}-1 & 0 & 0 & \ldots & 0\\ -1 & \lambda & -1 & \ldots & 0\\ 0 & -1 & \lambda & \ldots & 0\\ 0 & 0 & -1 & \ldots & 0\\ \vdots & \vdots & \vdots & \ldots & \vdots\\ 0 & 0 & 0 & \ldots & \lambda\end{vmatrix}_{k-2}$$

$= \lambda^2 \chi(Pk{-}2) - \lambda\, \chi(Pk{-}3) - \chi(Pk{-}2) - \chi(Pk{-}3) - \chi(Pk{-}3) - \lambda\, \chi(Pk{-}3)$

$= (\lambda^2 - 1)\, \chi(P_{k-2}) - 2(\lambda + 1)\, \chi(P_{k-3})$,

where $\chi(P_{k-2})$ and $\chi(P_{k-3})$ are the characteristic polynomials of the paths P_{k-2} and P_{k-3} containing $k-2$ and $k-3$ vertices respectively.

In view of (1), to find the coefficient of λ^i in $\chi(G'_{1,k};\lambda)$, we find the coefficients of λ^{i-2} and λ^i in $\chi(P_{k-2})$ and the coefficients of λ^{i-1} and λ^i in $\chi(P_{k-3})$. We make use of the following characteristic polynomial of the path P_n:

$$\chi(P_n)=\sum_{t=0}^{\lfloor \frac{n}{2}\rfloor}(-1)^t\binom{n-t}{t}\lambda^{n-2t} \qquad (3)$$

Put $n = k - 2$ in (3). If $t = \frac{k-i}{2}$, then $n - 2t = i - 2$, and so the coefficient of λ^{i-2} in $\chi(P_{k-2})$ is $(-1)^{\frac{k-i}{2}}\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}}$, since, $n - t = k - 2 - \left(\frac{k-i}{2}\right) = \frac{k+i-4}{2}$. Again by putting $n = k - 2$ in (3), we obtain the coefficient of λ^i in $\chi(P_{k-2})$

to be $(-1)^{\frac{k-i-2}{2}}\binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}$ by taking $t=\frac{k-i-2}{2}$ as $n-2t=k-2-2\left(\frac{k-i-2}{2}\right)=i$ and $n-t=k-2-\left(\frac{k-i-2}{2}\right)=\frac{k+i-2}{2}$.

Similarly, by putting $n = k - 3$ and taking $t=\frac{k-i-2}{2}$ in (3), we see that the coefficient of λ^{i-1} in $\chi(P_{k-3})$ is $(-1)^{\frac{k-i-2}{2}}\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}$ Further putting $n = k - 3$ in (3), we see that the coefficient of λ^i in $\chi(P_{k-3})$ is $(-1)^{\frac{k-i-3}{2}}\binom{\frac{k+i-3}{2}}{\frac{k-i-3}{2}}$ by taking $t=\frac{k-i-3}{2}$.

Now by (1), we have,

{Coefficient of λ^i in $\chi(G'_{1,k};\lambda)$} =
{Coefficient of λ^{i-2} in $\chi(P_{k-3})$} − {Coefficient of λ^{i-2} in $\chi(P_{k-2})$} − 2{Coefficient of λ^{i-1} in $\chi(P_{k-3})$} − 2 {Coefficient of λ^i in $\chi(P_{k-3})$}.

Thus the coefficient of λ^i in $\chi(G'_{1,k})$ is given by

$$(-1)^{\frac{k-i}{2}}\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}}-(-1)^{\frac{k-2-i}{2}}\binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}-2\left[(-1)^{\frac{k-i-2}{2}}\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+(-1)^{\frac{k-i-3}{2}}\binom{\frac{k+i-3}{2}}{\frac{k-i-3}{2}}\right]$$

$$=\ (-1)^{\frac{k-i}{2}}\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}}+(-1)^{\frac{k-i}{2}}\binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}+2(-1)^{\frac{k-i}{2}}\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-3}{2}}{\frac{k-i-3}{2}}$$

$$=\ (-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}\right]+2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-3}{2}}{\frac{k-i-3}{2}}. \qquad \square$$

We make use of the following well known result for computing the characteristic polynomial of some graphs in Corollary 2.3.

Theorem 2.2: [1] Let v_1 be a vertex of degree 1 in the graph G and let v_2 be the vertex adjacent to v_1. If G_1 be the induced subgraph obtained from G by deleting the vertex v_1 and let G_2 be the induced subgraph obtained from G by deleting the vertices v_1 and v_2, then,

$$\chi(G;\lambda)=\lambda\,\chi(G_1;\lambda)-\chi(G_2;\lambda) \qquad (4)$$

Proof: See Theorem 2.11 in [1].
Corollary 2.3: Let $G'_{2,k}$, $G'_{3,k}$ and $G'_{4,k}$ be the graphs with k vertices as given below:

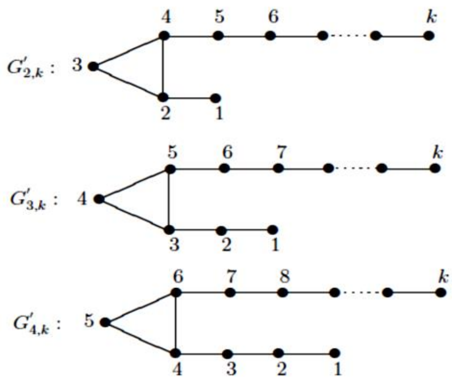

Fig. 2.2 Graphs $G'_{2,k}$, $G'_{3,k}$ and $G'_{4,k}$

Then, we have,

$$\chi(G'_{2,k}) = \lambda\, \chi(G'_{1,k-1}) - \chi(P_{k-2}) \quad (5)$$

$$\chi(G'_{3,k}) = \lambda\, \chi(G'_{2,k-1}) - \chi(G'_{1,k-2}) \quad (6)$$

$$\chi(G'_{4,k}) = \lambda\, \chi(G'_{3,k-1}) - \chi(G'_{2,k-2}) \quad (7)$$

Theorem 2.4: The coefficient of λ^i in $\chi(G'_{2,k})$ is

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}} + \binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}\right] + 2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-5}{2}}{\frac{k-i-3}{2}} \quad (8)$$

In the above, when $k-i \equiv 1 (\mathrm{mod}\ 2)$, the first sum vanishes and when $k \equiv i (\mathrm{mod}\ 2)$, second sum vanishes.

Proof: By Corollary 2.3, we have $\chi(G'_{2,k}) = \lambda\, \chi(G'_{1,k-1}) - \chi(P_{k-2})$. Thus, the coefficient of λ^i in $\chi(G'_{2,k}) =$

{Coefficient of λ^{i-1} in $\chi(G'_{1,k-1})$} - {Coefficient of λ^i in $\chi(P_{k-2})$}.

By putting $i = i-1$ and $k = k-1$ in Theorem 2.1, we obtain the coefficient of of λ^{i-1} in $\chi(G'_{1,k-1})$ to be:

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}\right] + 2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-5}{2}}{\frac{k-i-3}{2}}.$$

Also, by (3), the coefficient of λ^i in $\chi(P_{k-2})$ is $(-1)^{\frac{k-i-2}{2}}\binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}$.

Therefore the coefficient of λ^i in $\chi(G'_{2,k})$ is given by,

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}\right] + 2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-5}{2}}{\frac{k-i-3}{2}} - (-1)^{\frac{k-i-2}{2}}\binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}$$

$$= (-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}\right] + 2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-5}{2}}{\frac{k-i-3}{2}}$$

$$= (-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}} + \binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}\right]$$

$$+2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-5}{2}}{\frac{k-i-3}{2}}$$

$$= (-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}} + \binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}\right] + 2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-5}{2}}{\frac{k-i-3}{2}}$$

Theorem 2.5: The coefficient of λ^i in $\chi(G'_{3,k})$ is

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\right]$$

$$+2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}} + \binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}\right]. \quad (9)$$

In the above, when $k-i \equiv 1 (\mathrm{mod}\ 2)$, the first sum vanishes and when $k \equiv i (\mathrm{mod}\ 2)$, second sum vanishes.

Proof: By Corollary 2.3, we have, $(G'_{3,k}) = \lambda\, \chi(G'_{2,k-1}) - \chi(G'_{1,k-2})$.

Thus, the coefficient of λ^i in $\chi(G'_{3,k})$ is

{Coefficient of λ^{i-1} in $\chi(G'_{2,k-1})$} - {Coefficient of λ^i in $\chi(G'_{1,k-2})$}.

By putting $i = i-1$, $k = k-1$ in Theorem 2.4, the coefficient of λ^{i-1} in $\chi(G'_{2,k})$ is seen to be

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}\right]+2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}}.$$

Also by replacing k by $k-2$ in the Theorem 2.1, we obtain the coefficient of λ^i
In $\chi(G'_{1,k})$:

$$(-1)^{\frac{k-i-2}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}+\right]+2(-1)^{\frac{k-i-3}{2}}\binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}.$$

Therefore the coefficient of λ^i in $\chi(G'_{3,k})$ is given by

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}\right]+2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}}$$

$$-(-1)^{\frac{k-i-2}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}+\right]-2(-1)^{\frac{k-i-3}{2}}\binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}$$

$$=\ (-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}\right]+2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}}$$

$$+(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}+\right]+2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}$$

$$=\ (-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}\right.$$

$$\left.+2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\right]+2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}}+\binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}\right].$$

Theorem 2.6: The coefficient of λ^i in $\chi(G'_{4,k})$ is given by

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-8}{2}}{\frac{k-i}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-10}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\right.$$

$$\left.+3\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}\right]+2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}}+2\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}\right]. \qquad (10)$$

In the above, when $k - i \equiv 1 \pmod 2$, the first sum vanishes and when $k \equiv i \pmod 2$, second sum vanishes.

Proof: By Corollary 2.3, we have, $\chi(G'_{4,k}) = \lambda\,\chi(G'_{3,k-1}) - \chi(G'_{2,k-2})$.
Thus, the coefficient of λ^i in $\chi(G'_{4,k}) =$

{Coefficient of λ^{i-1} in $\chi(G'_{3,k-1})$} $-$ {Coefficient of λ^i in $\chi(G'_{2,k-2})$}.

By putting $i = i-1$, $k = k-1$ in Theorem 2.5, the coefficient of λ^{i-1} in $\chi(G'_{3,k})$is seen to be

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-8}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-10}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}+2\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}\right]$$

$$+2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}}+\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}\right].$$

By replacing k by $k-2$ in the Theorem 2.4, we obtain the coefficient of λ^i in $\chi(G'_{2,k})$:

$$(-1)^{\frac{k-i-2}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}\right]+2(-1)^{\frac{k-i-3}{2}}\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}.$$

Therefore the coefficient of λ^i in $\chi(G'_{4,k})$ is given by

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-8}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-10}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}+2\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}\right]$$
$$+2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}}+\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}\right]$$
$$-(-1)^{\frac{k-i-2}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}\right]-2(-1)^{\frac{k-i-3}{2}}\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}$$

$$= (-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-8}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-10}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\right.$$
$$\left.+2\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}\right]+2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}}+\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}\right]+(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}\right.$$
$$\left.+\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}\right]+2(-1)^{\frac{k-i-1}{2}}\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}$$
$$= (-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-8}{2}}{\frac{k-i}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-10}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\right.$$
$$\left.+3\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}\right]+2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}}+2\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}\right].$$

Theorem 2.7: For any graph G, let $b_i(G) = |a_i(G)|$, where $a_i(G)$ is the coefficient λ^i in $\chi(G;\lambda)$. Then,

$$b_i(G'_{1,k}) \geq b_i(G'_{3,k}) \geq b_i(G'_{4,k}) \geq b_i(G'_{2,k}).$$

Proof: We prove that:

(i) $b_i(G'_{1,k}) \geq b_i(G'_{3,k})$,

(ii) $b_i(G'_{3,k}) \geq b_i(G'_{4,k})$,

(iii) $b_i(G'_{4,k}) \geq b_i(G'_{2,k})$.

Proof of (i): We have two cases to be considered.

Suppose i and k are not of same parity. Note that the coefficient of λ^i in $\chi(G'_{1,k})$ is given in equation (2) and the coefficient of λ^i in $\chi(G'_{3,k})$ is given in equation (9). Also, note that when i and k are not of same parity, the first sum in (2) and (9) vanish and so we need to consider only the second sum $(-1)^{\frac{k-i-1}{2}}2\binom{\frac{k+i-3}{2}}{\frac{k-i-3}{2}}$ of (2) and the second sum $(-1)^{\frac{k-i-1}{2}}2\left[\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}}+\binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}\right]$ of (9).

Using the binomial identity:

$$\binom{n}{r}=\binom{n-1}{r}+\binom{n-1}{r-1},$$

we expand above sums to obtain:

$$\begin{aligned}\binom{\frac{k+i-3}{2}}{\frac{k-i-3}{2}} &= \binom{\frac{k+i-5}{2}}{\frac{k-i-3}{2}}+\binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}\\ &= \binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}}+\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}+\binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}\\ &= \left[\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}}+\binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}\right]+\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}.\end{aligned}$$

Thus, in this case we observe that $b_i(G'_{1,k}) \geq b_i(G'_{3,k})$.

Suppose *i* and *k* are of same parity. Note that when *i* and *k* are of same parity, the second sum in equation (2) and equation (9) vanish and so we need to consider

only the first sum $(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}\right]$ of (2) and the first

sum

$$(-1)^{\frac{k-i}{2}}\left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\right]$$

of (9).

Again by using the binomial identity, we have,

$$\begin{aligned}&\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}\\ &= \left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}\right]+\left[\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}\right]\\ &\quad+\left[\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}\right]\\ &= \left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}\right]+\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\\ &= \left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}\right]+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\\ &\quad+\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\end{aligned}$$

$$\begin{aligned}
&= \left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\right] + \binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} \\
&= \left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}\right] + \binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}} \\
&\quad + \binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}} \\
&= \left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}} + \binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}\right] \\
&\quad + \binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}.
\end{aligned}$$

Thus we see that: $\boldsymbol{b_i(G'_{1,k}) \geq b_i(G'_{3,k})}$. This proves (i).

Proof of (ii):

We show that $\boldsymbol{b_i(G'_{3,k})} \geq b_i(\boldsymbol{G'_{4,k}})$. For this we consider two cases.

Suppose i and k are not of same parity. Note that the coefficient of λ^i in $\boldsymbol{\chi(G'_{3,k})}$ is given in equation (9), and the coefficient of λ^i in $\boldsymbol{\chi(G'_{4,k})}$ is given in equation (10). Also note that when i and k are not of same parity, the first sum in (9) and (10) vanish and so we need to consider only the second sum $\boldsymbol{2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}} + \binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}\right]}$ of (9) and the second sum $\boldsymbol{2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}} + \binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}\right]}$ of (10).

Consider the term $\boldsymbol{\left[\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}} + \binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}}\right]}$. By putting $\boldsymbol{\frac{k+i-1}{2} = r}$ and $\boldsymbol{\frac{k-i-1}{2} = s}$,

we obtain by using the binomial identity,

$$\begin{aligned}
\binom{\frac{k+i-7}{2}}{\frac{k-i-3}{2}} + \binom{\frac{k+i-5}{2}}{\frac{k-i-5}{2}} &= \binom{r-3}{s-1} + \binom{r-2}{s-2} \\
&= \left[\binom{r-4}{s-1} + \binom{r-4}{s-2}\right] + \left[\binom{r-3}{s-2} + \binom{r-3}{s-3}\right] \\
&= \left[\binom{r-4}{s-1} + \binom{r-3}{s-2}\right] + \binom{r-4}{s-2} + \left[\binom{r-4}{s-3} + \binom{r-4}{s-4}\right] \\
&= \left[\binom{r-4}{s-1} + \binom{r-3}{s-2}\right] + \left\{\binom{r-4}{s-2} + \binom{r-4}{s-3}\right\} + \binom{r-4}{s-4} \\
&= \left[\binom{r-4}{s-1} + \binom{r-3}{s-2}\right] + \binom{r-3}{s-2} + \binom{r-4}{s-4} \\
&= \left[\binom{r-4}{s-1} + 2\binom{r-3}{s-2}\right] + \binom{r-4}{s-4} \\
&= \left[\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}} + 2\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}\right] + \binom{\frac{k+i-9}{2}}{\frac{k-i-9}{2}}
\end{aligned}$$

Hence, $\boldsymbol{b_i(G'_{3,k}) \geq b_i(G'_{4,k})}$.

Suppose i and k are of same parity. Note that when i and k are of same parity, the second sum in equation (9) and equation (10) vanish and so we need to consider only the first sum

$$A = \left[\binom{\frac{k+i-6}{2}}{\frac{k-i}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}} + \binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}\right]$$

of (9) and the first sum

$$B = \left[\binom{\frac{k+i-8}{2}}{\frac{k-i}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}} + \binom{\frac{k+i-10}{2}}{\frac{k-i-2}{2}} + 2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}} + 3\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}} + \binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}\right]$$

of (10). We need to show that $A-B \geq 0$. By substituting $\boldsymbol{\frac{k+i}{2} = r}$ and $\boldsymbol{\frac{k-i}{2} = s}$,
we get,

$$A = \binom{r-3}{s} + \binom{r-2}{s-1} + 2\binom{r-3}{s-1} + \binom{r-4}{s-1} + \binom{r-2}{s-2} + 2\binom{r-3}{s-2}$$

$$B = \binom{r-4}{s} + 2\binom{r-3}{s-1} + 2\binom{r-4}{s-1} + \binom{r-5}{s-1} + 2\binom{r-3}{s-2} + 3\binom{r-4}{s-2} + \binom{r-2}{s-2}$$

Consider

$$\begin{aligned}
A - B &= \binom{r-3}{s} + \binom{r-2}{s-1} + 2\binom{r-3}{s-1} + \binom{r-4}{s-1} + \binom{r-2}{s-2} + 2\binom{r-3}{s-2} \\
&\quad - \binom{r-4}{s} - 2\binom{r-3}{s-1} - 2\binom{r-4}{s-1} - \binom{r-5}{s-1} - 2\binom{r-3}{s-2} \\
&\quad - 3\binom{r-4}{s-2} - \binom{r-2}{s-2} \\
&= \binom{r-3}{s} + \binom{r-2}{s-1} - \binom{r-4}{s-1} - \binom{r-4}{s} - \binom{r-5}{s-1} - 3\binom{r-4}{s-2} \\
&= \left[\binom{r-4}{s} + \binom{r-4}{s-1}\right] + \binom{r-2}{s-1} - \binom{r-4}{s-1} - \binom{r-4}{s} - \binom{r-5}{s-1} \\
&\quad - 3\binom{r-4}{s-2} \\
&= \binom{r-2}{s-1} - \binom{r-5}{s-1} - 3\binom{r-4}{s-2} \\
&= \binom{r-2}{s-1} - \binom{r-5}{s-1} - \left[\binom{r-5}{s-2} + \binom{r-5}{s-3}\right] - 2\binom{r-4}{s-2} \\
&= \binom{r-2}{s-1} - \left[\binom{r-5}{s-1} + \binom{r-5}{s-2}\right] - \binom{r-5}{s-3} - 2\binom{r-4}{s-2} \\
&= \binom{r-2}{s-1} - \binom{r-4}{s-1} - \binom{r-5}{s-3} - 2\binom{r-4}{s-2}
\end{aligned}$$

$$= \binom{r-2}{s-1} - \left[\binom{r-4}{s-1} + \binom{r-4}{s-2}\right] - \binom{r-5}{s-3} - \binom{r-4}{s-2}$$
$$= \binom{r-2}{s-1} - \binom{r-3}{s-1} - \binom{r-5}{s-3} - \binom{r-4}{s-2}$$
$$= \binom{r-3}{s-1} + \binom{r-3}{s-2} - \binom{r-3}{s-1} - \binom{r-5}{s-3} - \binom{r-4}{s-2}$$
$$= \binom{r-3}{s-2} - \binom{r-5}{s-3} - \binom{r-4}{s-2}$$
$$= \binom{r-4}{s-2} + \binom{r-4}{s-3} - \binom{r-5}{s-3} - \binom{r-4}{s-2}$$
$$= \binom{r-5}{s-3} + \binom{r-5}{s-4} - \binom{r-5}{s-3}.$$
$$= \binom{r-5}{s-4} \geq 0.$$

Thus $A - B \geq 0$, proving there by that $\boldsymbol{b_i(G'_{3,k}) \geq b_i(G'_{4,k})}$.

Proof of (iii): Finally we show $\boldsymbol{b_i(G'_{4,k}) \geq b_i(G'_{2,k})}$. Again there are two cases to be considered.

Suppose i and k are not of same parity. Note that the coefficient of λ^i in $\boldsymbol{\chi(G'_{4,k})}$ is given in equation (10) and the coefficient of λ^i in $\boldsymbol{\chi(G'_{2,k})}$ is given in equation (8). Also note that when i and k are not of same parity, the first sum in (10) and in (8) vanish and so we need to consider only the second sum $\boldsymbol{2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}} + 2\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}\right]}$ of (10) and the second term $\boldsymbol{2(-1)^{\frac{k-i-1}{2}}\left[\binom{\frac{k+i-5}{2}}{\frac{k-i-3}{2}}\right]}$ of (8).

Consider the term $\boldsymbol{\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}} + 2\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}}}$. By putting $\boldsymbol{\frac{k+i-1}{2} = r}$ and $\boldsymbol{\frac{k-i-1}{2} = s}$, we get,

$$\binom{\frac{k+i-9}{2}}{\frac{k-i-3}{2}} + 2\binom{\frac{k+i-7}{2}}{\frac{k-i-5}{2}} = \binom{r-4}{s-1} + 2\binom{r-3}{s-2}$$
$$= \binom{r-4}{s-1} + \left[\binom{r-4}{s-2} + \binom{r-4}{s-3}\right] + \binom{r-3}{s-2}$$
$$= \left[\binom{r-4}{s-1} + \binom{r-4}{s-2}\right] + \binom{r-4}{s-3} + \binom{r-3}{s-2}$$
$$= \binom{r-3}{s-1} + \binom{r-3}{s-2} + \binom{r-4}{s-3}$$
$$= \binom{r-2}{s-1} + \binom{r-4}{s-3}$$
$$= \left[\binom{\frac{k+i-5}{2}}{\frac{k-i-3}{2}}\right] + \binom{\frac{k+i-9}{2}}{\frac{k-i-7}{2}}.$$

Hence, $\boldsymbol{b_i}(\boldsymbol{G'_{4,k}}) \geq \boldsymbol{b_i}(\boldsymbol{G'_{2,k}})$.

Suppose *i* and *k* are of same parity. Note that when *i* and *k* are of same parity, the second sum in equation (10) and equation (8) vanish and so we need to consider only the first sum

$$B=\binom{\frac{k+i-8}{2}}{\frac{k-i}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-8}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-10}{2}}{\frac{k-i-2}{2}}+2\binom{\frac{k+i-6}{2}}{\frac{k-i-4}{2}}+3\binom{\frac{k+i-8}{2}}{\frac{k-i-4}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-4}{2}}$$

of (10) and the first sum $\boldsymbol{C}=\binom{\frac{k+i-4}{2}}{\frac{k-i}{2}}+\binom{\frac{k+i-2}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-4}{2}}{\frac{k-i-2}{2}}+\binom{\frac{k+i-6}{2}}{\frac{k-i-2}{2}}$ of (8).

By substituting $\frac{k+i}{2}=\boldsymbol{r}$ and $\frac{k-i}{2}=\boldsymbol{s}$, we get

$$\boldsymbol{B}=\binom{r-4}{s}+2\binom{r-3}{s-1}+2\binom{r-4}{s-1}+\binom{r-5}{s-1}+2\binom{r-3}{s-2}+3\binom{r-4}{s-2}+\binom{r-2}{s-2},$$

$$C=\binom{r-2}{s}+\binom{r-1}{s-1}+\binom{r-2}{s-1}+\binom{r-3}{s-1}.$$

Consider

$$\begin{aligned}
B-C &= \binom{r-4}{s}+2\binom{r-3}{s-1}+2\binom{r-4}{s-1}+\binom{r-5}{s-1}+2\binom{r-3}{s-2}+3\binom{r-4}{s-2}\\
&\quad+\binom{r-2}{s-2}-\binom{r-2}{s}-\binom{r-1}{s-1}-\binom{r-2}{s-1}-\binom{r-3}{s-1}\\
&= \left[\binom{r-4}{s}+\binom{r-4}{s-1}\right]+\binom{r-3}{s-1}+\binom{r-4}{s-1}+\binom{r-5}{s-1}+2\binom{r-3}{s-2}\\
&\quad+3\binom{r-4}{s-2}+\binom{r-2}{s-2}-\binom{r-2}{s}-\binom{r-1}{s-1}-\binom{r-2}{s-1}\\
&= \binom{r-3}{s}+\binom{r-3}{s-1}+\binom{r-4}{s-1}+\binom{r-5}{s-1}+2\binom{r-3}{s-2}+3\binom{r-4}{s-2}\\
&\quad+\binom{r-2}{s-2}-\left[\binom{r-3}{s}+\binom{r-3}{s-1}\right]-\left[\binom{r-2}{s-1}+\binom{r-2}{s-2}\right]-\binom{r-2}{s-1}\\
&= \binom{r-4}{s-1}+\binom{r-5}{s-1}+2\binom{r-3}{s-2}+3\binom{r-4}{s-2}-2\binom{r-2}{s-1}\\
&= \binom{r-4}{s-1}+\binom{r-5}{s-1}+2\binom{r-3}{s-2}+3\binom{r-4}{s-2}-2\left[\binom{r-3}{s-1}+\binom{r-3}{s-2}\right]\\
&= \binom{r-4}{s-1}+\binom{r-5}{s-1}+3\binom{r-4}{s-2}-2\binom{r-3}{s-1}\\
&= \binom{r-4}{s-1}+\binom{r-5}{s-1}+3\binom{r-4}{s-2}-2\left[\binom{r-4}{s-1}+\binom{r-4}{s-2}\right]\\
&= -\binom{r-4}{s-1}+\binom{r-5}{s-1}+\binom{r-4}{s-2}\\
&= -\binom{r-5}{s-1}-\binom{r-5}{s-2}+\binom{r-5}{s-1}+\binom{r-4}{s-2}\\
&= -\binom{r-5}{s-2}+\binom{r-5}{s-2}+\binom{r-5}{s-3}
\end{aligned}$$

$$= \binom{r-5}{s-3} \geq 0$$

Thus $B - C \geq 0$, proving there by that $b_i(G'_{4,k}) \geq b_i(G'_{2,k})$.
This proves the theorem.

Corollary 2.8: For $k \geq 6$, we have, $G'_{1,k} \geq G'_{3,k} \geq G'_{4,k} \geq G'_{2,k}$. Consequently,
$E(G'_{1,k}) \geq E(G'_{3,k}) \geq E(G'_{4,k}) \geq E(G'_{2,k})$.
Proof: The first statement follows from Theorem 2.7. The second statement follows from Theorem 1.3.

Remark 2.9: The characteristic polynomial and energy of the adjacency matrix of a unicyclic graphs $G'_{1,k}$, $G'_{2,k}$, $G'_{3,k}$ and $G'_{4,k}$ for $k = 7, 8, 9$ (by using *maple*) are given below:

No. of vertices k	Graphs	Characteristic Polynomial	Energy (approx.)
$k = 7$	$G'_{1,7}$	$\lambda^7 - 7\lambda^5 - 2\lambda^4 + 13\lambda^3 + 6\lambda^2 - 5\lambda - 2$	8.9405
	$G'_{3,7}$	$\lambda^7 - 7\lambda^5 - 2\lambda^4 + 12\lambda^3 + 4\lambda^2 - 5\lambda - 2$	8.8698
	$G'_{4,7}$	$\lambda^7 - 7\lambda^5 - 2\lambda^4 + 12\lambda^3 + 4\lambda^2 - 4\lambda$	8.4554
	$G'_{2,7}$	$\lambda^7 - 7\lambda^5 - 2\lambda^4 + 12\lambda^3 + 4\lambda^2 - 4\lambda$	8.4554
$k = 8$	$G'_{1,8}$	$\lambda^8 - 8\lambda^6 - 2\lambda^5 + 19\lambda^4 + 8\lambda^3 - 13\lambda^2 - 6\lambda + 1$	10.106
	$G'_{3,8}$	$\lambda^8 - 8\lambda^6 - 2\lambda^5 + 18\lambda^4 + 6\lambda^3 - 12\lambda^2 - 4\lambda + 1$	9.996
	$G'_{4,8}$	$\lambda^8 - 8\lambda^6 - 2\lambda^5 + 18\lambda^4 + 6\lambda^3 - 12\lambda^2 - 4\lambda + 1$	9.996
	$G'_{2,8}$	$\lambda^8 - 8\lambda^6 - 2\lambda^5 + 18\lambda^4 + 6\lambda^3 - 11\lambda^2 - 2\lambda + 1$	9.93
$k = 9$	$G'_{1,9}$	$\lambda^9 - 9\lambda^7 - 2\lambda^6 + 26\lambda^5 + 10\lambda^4 - 26\lambda^3 - 12\lambda^2 + 6\lambda + 2$	11.4701
	$G'_{3,9}$	$\lambda^9 - 9\lambda^7 - 2\lambda^6 + 25\lambda^5 + 8\lambda^4 - 24\lambda^3 - 8\lambda^2 + 6\lambda + 2$	11.3853
	$G'_{4,9}$	$\lambda^9 - 9\lambda^7 - 2\lambda^6 + 25\lambda^5 + 8\lambda^4 - 24\lambda^3 - 8\lambda^2 + 5\lambda$	11.0603
	$G'_{2,9}$	$\lambda^9 - 9\lambda^7 - 2\lambda^6 + 25\lambda^5 + 8\lambda^4 - 23\lambda^3 - 6\lambda^2 + 5\lambda$	11.0342

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