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Tripartite Graphs with Energy Aggregation

Nawras A. Alawn and Nadia M. G. Al-Saidi and Rashed T. Rasheed

ABSTRACT: The aggregate of the absolute values of the graph eigenvalues is called the energy of a graph. It is used to approximate the total π-electron energy of molecules. Thus, finding a new mechanism to calculate the total energy of some graphs is a challenge; it has received a lot of research attention. We study the eigenvalues of a complete tripartite graph $T_{i,i,n-2i}$, for $n \geq 4$, based on the adjacency, Laplacian, and signless Laplacian matrices. In terms of the degree sequence, the extreme eigenvalues of the irregular graphs energy are found to characterize the component with the maximum energy. The chemical HMO approach is particularly successful in the case of the total π-electron energy. We showed that some chemical components are equienergetic with the tripartite graph. This discovering helps easily to derive the HMO for most of these components despite their different structures.

Key Words: Spectrum, Tripartite graph, Adjacency matrix ($\mathcal{A}$), Laplacian matrix (L), Signless matrix (S), Characteristic polynomial (CH).

Contents

1. Introduction

Spectral graph theory is a branch of graph-theoretical emerged in the 50s, which study on the relationship between the structural and spectral properties of graphs, another major research was sourced in quantum chemistry. The relation between

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these subjects of work remained undiscovered until much later. The monograph spectra of the graphs by Cvetkovic et al. [1], summarized nearly all research in this area. This summary was updated by a survey of the recent theories of the spectral results of the graphs.

Spectrum has several applications in chemical, physics, medicine, computer science, information theory, geographic studies, and social sciences. Eigenvalues interact with a number of chemical topics, such as the total energy of π-electron in a molecule, which is the summation of eigenvalues. The membrane vibration problem can be addressed by approximating the solution of the corresponding partial differential equation that considers the eigenvalues of the graph, a discrete model of the membrane. Eigenvalues are widely used in various areas such as physics, particularly in statistical physics and thermodynamic [1]; furthermore, it has great importance in image processing especially in face recognition [2,3], as well as image clustering [4,5] and image segmentation [6]. Eigenvalues have also been applied in medical sciences, including the diagnosis of cancers by assigning a potential link between a pair of cells (cells or clusters) [7], as well as, the functional integration of environmental networks through the deployment path [8].

Let G be finite undirected simple connected graph, then $G(V,E)$ consists of two finite sets, the set of vertices V and the set of edges E, which contains the unordered pairs of vertices (v_i, v_j) [9]. The order G is the number of vertices n, such that $|V(G)| = n$, and the size of a graph G is the number m of edges such that, $|E(G)| = m$.

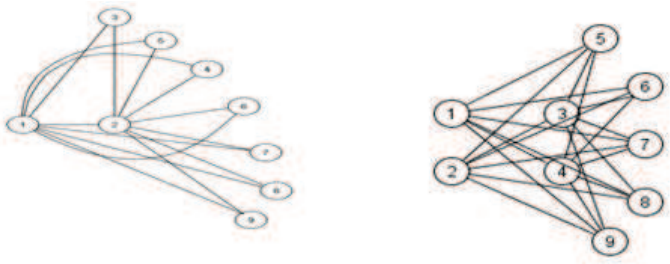
The degree of a vertex $d(v_i)$ or d_i is the number of edges incident to the vertex v_i. The maximum degree of a vertex in G is denoted by $\triangle(G) = \triangle$ and defined as $\triangle(G) = max\{d(v_i)|v_i \in V(G)\}$. Similarly, the minimum degree of a vertex in G, denoted by $\eta(G) = \eta$, is defined by $\eta(G) = min\{d(v_i)|v_i \in V(G)\}$.

The adjacency matrix $\mathcal{A}(G)$ is defined by $0, 1$, whose (i, j) entry is 1 if $(v_i, v_j) \in E$, and 0 otherwise [9]. The set of $\mathcal{A}(G)$ eigenvalues are denoted by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Let $D(G) = \{d_1, d_2, d_3, \cdots, d_n\}$ be the matrix which contains the degree of each vertex. It is called the degree matrix of G. The Laplacian matrix of G is $L(G) = D(G) - \mathcal{A}(G)$, where $L(G)$ is a real symmetric matrix and its eigenvalues are; $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. The signless Laplacian matrix of G is defined by $S(G) = D(G) + \mathcal{A}(G)$, where its eigenvalues are $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$.

The complete tripartite graph $T_{i,i,n-2i}$ [10] consists of three sets of vertices sized i, i and $n - 2i$, where n is the number of all vertices. Their edges are defined, if and only if, they lie in different sets. Figure 1 shows the complete tripartite graphs $T_{1,1,7}$ and $T_{2,2,5}$.

The tripartite graph plays an important role in several applications, including chemistry, where some molecular orbital for chemistry compounds can be represented by the tripartite graph. For example, octahedral can be represented by $T_{2,2,2}$, whereas dyck can be represented by the symmetrical tripartite graph $T_{4,4,4}$ and other [11]. Therefore, some researchers pay considerable attention to this graph. In 1980, Cvetkovic et al. [1] introduced the characteristic polynomial of the complete multiple graph $T_{n_1,n_2,\ldots,n_p}$. In 2012, Delorme [12] first presented another general formula of the characteristic polynomial of the complete multiple

graph $T_{p_1,p_2,\ldots,p_k}$.
In this article, the spectrum of the graph is introduced, and general formulas are constructed based on adjacency, Laplacian, and signless Laplacian matrices. The extreme eigenvalues (maximum and minimum eigenvalues) are also demonstrated. In 2003, Stevanovic [13] introduced a new formula for the largest eigenvalue of the connected irregular graph G.
In this work, a new formula of extreme eigenvalues for some connected irregular complete tripartite graph is used based on the number of vertices and the maximum degree Δ. This formula is compared with the Stevanovic [13] and Zhang's [14] formula.



(a) $T_{1,1,7}$ (b) $T_{2,2,5}$

Figure 1: Complete tripartite graphs $T_{1,1,7}$,$T_{2,2,5}$

2. Primary Concepts

Properties of $\mathbf{T_{i,i,n-2i}}$:

1. The number of cycle C with length 3 in $T_{i,i,n-2i}$ is equal $i(n-2i)$.

   Proof. Since $T_{i,i,n-2i}$ has three sets of vertices and each cycle has length 3, the number of cycle depends on the number of the third set of vertices sized $(n-2i)$ multiplied by i, as shown in Figure 2.

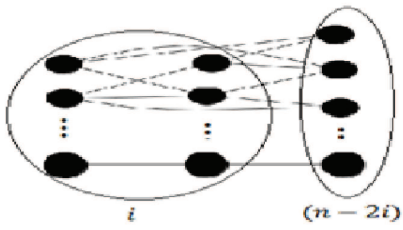


Figure 2: Number of cycles of length 3

□

2. The number of edges in $T_{i,i,n-2i}$ is given by:

$$|E(T_{i,i,n-2i})| = i((n-2i)+i) + i(n-2i)$$

The proof is trivial.

3. The eigenvalues of $T_{i,i,n-2i}$ based on adjacency matrix $\mathcal{A}$

In this section, we introduced the general form of the eigenvalues of $T_{i,i,n-2i}$ based on adjacency matrix $\mathcal{A}$ and some properties of it.

Theorem 3.1. *Let $T_{i,i,n-2i}$ be a simple connected non-regular graph of order n and m be the size of $T_{i,i,n-2i}$. Then the general formula of eigenvalues of $T_{i,i,n-2i}$ based on adjacency matrix $\mathcal{A}$ is given by*

$$\left\{0^3, -i, \frac{i+\sqrt{i^2+4g}}{2}, \frac{i-\sqrt{i^2+4g}}{2}\right\}. \tag{3.1}$$

Proof. The eigenvalues of any graph can be found by solving its characteristic polynomial. The adjacency matrix-based characteristic polynomial of G is refereed to as $CH(\mathcal{A}, G)$, such that; $CH(\mathcal{A}, G) = |\mathcal{A} - \lambda I|$ and it is computed by letting $|\mathcal{A} - \lambda I| = 0$. For $T_{i,i,n-2i}$, the characteristic polynomial is obtained by computing the determinant of

$$|\mathcal{A}(T_{i,i,n-2i}) - \lambda I| = 0,$$

and given in equation (3);

$$CH(\mathcal{A}, T_{i,i,n-2i}) = \begin{vmatrix} -\lambda & 0 & \cdots & 0 & 1 & \cdots & \cdots & \cdots & \cdots & \cdots & 1 \\ 0 & \ddots & \ddots & \vdots & \vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \vdots \\ \vdots & \ddots & -\lambda & 0 & \vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \vdots \\ 0 & \cdots & 0 & -\lambda & 1 & \cdots & \cdots & \cdots & \cdots & \cdots & 1 \\ 1 & \cdots & \cdots & 1 & -\lambda & 0 & \cdots & 0 & 1 & \cdots & 1 \\ \vdots & \cdots & \cdots & \vdots & 0 & \ddots & \ddots & \vdots & \vdots & \cdots & \vdots \\ 1 & \cdots & \cdots & 1 & \vdots & \ddots & -\lambda & 0 & 1 & \cdots & 1 \\ 1 & \cdots & \cdots & 1 & 0 & \cdots & 0 & -\lambda & 1 & \cdots & 1 \\ 1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 1 & -\lambda & 0 & 0 \\ \vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & \ddots & \vdots \\ \vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \vdots & \ddots & 0 \\ 1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 1 & 0 & \cdots & -\lambda \end{vmatrix}. \tag{3.2}$$

Therefore,

$$CH(\mathcal{A}, T_{i,i,n-2i}) = \lambda^n - (i^2 + (2i(n-2i)))\lambda^{n-2} - (2i^2(n-2i))\lambda^{(n-3)}. \tag{3.3}$$

The eigenvalues are obtained when $CH(\mathcal{A}, T_{i,i,n-2i}) = 0$, such that

$$\lambda^n - (i^2 + (2i(n-2i)))\lambda^{n-2} - (2i^2(n-2i))\lambda^{(n-3)} = 0. \tag{3.4}$$

Then, after some simplification, we have

$$\lambda^{n-3}(\lambda^3 - (i^2 + (2i(n-2i)))\lambda - (2i^2(n-2i))) = 0. \tag{3.5}$$

Therefore, from the first part of the equation (3.5), we have $(n-3)$ of the eigenvalues are equal to zero, and the second part of the equation (3.5) given in the equation (3.6) is also equal to zero, such that

$$(\lambda^{n-3}(\lambda + i)(\lambda^2 - 2i\lambda) - \frac{(2i^2(n-2i))}{i}) = 0. \tag{3.6}$$

By solving the equation (3.6), the set of eigenvalues can be found

$$\left\{0^3, -i, \frac{i + \sqrt{i^2 + 4g}}{2}, \frac{i - \sqrt{i^2 + 4g}}{2}\right\} \tag{3.7}$$

where $g = \frac{(2i^2(n-2i))}{i}$.
□

Theorem 3.2. *Let $T_{i,i,n-2i}$ be a simple connected non-regular graph of order n and m be the size of $T_{i,i,n-2i}$. Then the eigenvalues of $T_{i,i,n-2i}$ have some properties;*

1. $\lambda_1 = |\lambda_n + i|$,
2. $\lambda_1 < n$,
3. $\lambda_n \leq 0$,
4. *In general for $i = 1, 2, 3, \cdots$, the eigenvalues are*

$$\lambda_1(T_{1,1,n-2}) \leq \lambda_1(T_{2,2,n-4}) \leq \lambda_1(T_{3,3,n-6}) \leq \cdots. \tag{3.8}$$

Proof. 1. Since $\sum_{i=1}^{n} \lambda_i = 0$, [1], by applying of this relation to the set of the eigenvalues of $T_{i,i,n-2i}$, we obtained

$$\lambda_1 - \lambda_n - i = 0. \tag{3.9a}$$

Then

$$\lambda_1 = \lambda_n + i \qquad where \quad \lambda_n \leq 0. \tag{3.9b}$$

Consequently

$$\lambda_1 = |\lambda_n + i|.$$

2. It is obvious from (1) that $\lambda_1 < n$ for $i \geq 1$ and $n \geq 1$.

3. The proof of this property is similar to the proof of the second property.

4. Since

$$\lambda_1(T_{i-1,i-1,n-2(i-1)}) = \frac{i-1+\sqrt{(i-1)^2+4(\frac{(2(i-1)((i-1)(n-2(i-1))))}{i-1})}}{2}$$

where $i \geq 2$ and

$$\lambda_1(T_{i,i,n-2i}) = \frac{i+\sqrt{i^2+4(\frac{(2i(i(n-2i)))}{i})}}{2},$$

then

$$\lambda_1(T_{i-1,i-1,n-2(i-1)}) \leq \lambda_1(T_{i,i,n-2i}).$$

□

Table 1 shows some eigenvalues of $T_{i,i,n-2i}$ for $i = 2, 4, 5$.

i	n	$T_{i,i,n-2i}$
2	5	-1.2360, -2, 0, 0, 3.2360
	6	-2, -2, 0, 0, 0, 4
	7	-2.6056,-2,0,0,0,0,4.6056
	8	-3.1231,-2,0,0,0,0,0,5.1231
i	n	$T_{i,i,n-2i}$
4	9	$-1.4641, -4, 0^6, 5.4641$
	10	$-2.4721, -4, 0^7, 6.4721$
	11	$-3.2915, -4, 0^8, 7.2915$
	12	$-4, -4, 0^9, 8$
i	n	$T_{i,i,n-2i}$
5	11	$-1.5311, -5, 0^7, 6.5311$
	12	$-2.6235, -5, 0^8, 7.6235$
	13	$3.5208, -5, 0^9, 8.5208$
	16	$5.6394, -5, 0^13, 10.6394$

Table 1: The eigenvalues for some $T_{i,i,n-2i}$ based on $\mathcal{A}(T_{i,i,n-2i})$.

4. The eigenvalues of $T_{i,i,n-2i}$ based on Laplacian matrix L

In this section, we introduced the general form of the eigenvalues of $T_{i,i,n-2i}$ based on Laplacian matrix L and some properties of it.

Theorem 4.1. *Let $T_{i,i,n-2i}$ be a simple connected non-regular graph of order n and m be the size of $T_{i,i,n-2i}$. Then the general formula of eigenvalues of $T_{i,i,n-2i}$ based on Laplacian matrix L is given by*

$$\{0, n^2, (n-i)^{2i-2}, (2i)^{(n-2i)-1}\}. \tag{4.1}$$

Proof. The eigenvalues of any graph can be found by solving its characteristic polynomial. The characteristic polynomial of G based on Laplacian matrix is refereed to as $CH(L, G)$ such that,

$$CH(L, G) = |L - \lambda I| = 0.$$

For $T_{i,i,n-2i}$, the characteristic polynomial is obtained by computing the determinant of $|L(T_{i,i,n-2i}) - \lambda I|$ which is equal to zero and the determinant can be shown in (4.2) as

$$|L(T_{i,i,n-2i}) - \lambda I| =$$

$$\begin{vmatrix}
i+(n-2i)-\lambda & 0 & \cdots & 0 & -1 & \cdots & \cdots & -1 & \cdots & \cdots & \cdots & -1 \\
0 & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & & & & \vdots \\
\vdots & \ddots & i+(n-2i)-\lambda & 0 & \vdots & \vdots & \vdots & \vdots & \cdots & \cdots & \cdots & \vdots \\
0 & \cdots & 0 & i+(n-2i)-\lambda & -1 & \cdots & -1 & -1 & \cdots & \cdots & \cdots & -1 \\
-1 & \cdots & \cdots & -1 & i+(n-2i)-\lambda & 0 & \cdots & 0 & -1 & \cdots & \cdots & -1 \\
\vdots & \vdots & \vdots & \vdots & 0 & \ddots & \ddots & \vdots & \vdots & \cdots & \cdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & i+(n-2i)-\lambda & 0 & \vdots & \cdots & \cdots & \vdots \\
-1 & \cdots & \cdots & -1 & 0 & \cdots & 0 & i+(n-2i)-\lambda & -1 & \cdots & \cdots & -1 \\
-1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & -1 & 2i-\lambda & 0 & \cdots & 0 \\
\vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \vdots & 0 & \ddots & \ddots & \vdots \\
\vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \vdots & \vdots & \ddots & 2i-\lambda & \vdots \\
-1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & -1 & 0 & \cdots & 0 & 2i-\lambda
\end{vmatrix}. \tag{4.2}$$

After calculating of this determinant, we obtained,

$$(\mu)(\mu - n)^2(\mu - (n-i))^{2i-2}(\mu - 2i)^{(n-2i)-1} = 0. \tag{4.3}$$

Therefore, the spectrum of $T_{i,i,n-2i}$ is given in the following set

$$\{0, n^2, (n-i)^{2i-2}, (2i)^{(n-2i)-1}\}. \tag{4.4}$$

□

Table 2 shows some results for $i = 1, 4, 5$.

n	$T_{1,1,n-2}$	n	$T_{4,4,n-8}$	n	$T_{5,5,n-10}$
4	$0,2,4,4$	9	$0,9^2,5^6$	11	$0,11^2,6^8$
5	$0,2,2,5,5$	10	$0,10^2,6^6,8$	12	$0,12^2,7^6,10$
6	$0,2,2,2,6,6$	11	$0,11^2,7^6,8^2$	13	$0,13^2,8^6,10^2$
7	$0,2,2,2,2,7,7$	12	$0,12^2,8^6,8^3$	14	$0,14^2,9^6,10^2$
8	$0,2,2,2,2,2,8,8$	13	$0,13^2,9^6,8^4$	15	$0,15^2,10^6,10^2$

Table 2: The spectrum of $T_{1,1,n-2}$, $T_{4,4,n-8}$ and $T_{5,5,n-10}$ based on $\mathcal{L}(T_{i,i,n-2i})$

To simplify, based on Laplacian matrix, some properties of the spectrum of $T_{i,i,n-2i}$ are given as follows

- $\mu_1 = \mu_2 = n$,
- $\mu_2 = 0$,
- $\mu_i \geq 0$.

The proofs of these three properties can be easily calculated from the general spectral formula of $T_{i,i,n-2i}$ based on $\mathcal{L}(T_{i,i,n-2i})$.

5. The eigenvalues of $T_{i,i,n-2i}$ based on signless Laplacian matrix S

In this section, we introduced the general form of the eigenvalues of $T_{i,i,n-2i}$ based on signless Laplacian matrix S and some properties of it.

Theorem 5.1. *Let $T_{i,i,n-2i}$ be a simple connected non-regular graph of order n and m be the size of $T_{i,i,n-2i}$. Then the general formula of eigenvalues of $T_{i,i,n-2i}$ based on signless Laplacian matrix S is given by*

$$\{n-2i, (n-i)^{(2i-2)}, (2i)^{(n-2i)-1}, \frac{B+C}{2}, \frac{B-C}{2}\} \tag{5.1}$$

where $B = (a_1) - (\delta_2 + \delta_3 + \delta_4)$, $C = \sqrt{B^2 - 4z_3}$,
and $a_1 = (2i^2 + 2i(n-2i)) + (2i(n-2i))$.

Proof. The eigenvalues of any graph can be found by solving its characteristic polynomial. The characteristic polynomial of G based on signless matrix is refereed to as $CH(S,G)$ such that,

$$CH(S,G) = |S - \lambda I| = 0.$$

For $T_{i,i,n-2i}$, the characteristic polynomial is obtained by computing the determinant of $|S(T_{i,i,n-2i}) - \lambda I|$ which is equal to zero and the signless matrix of $T_{i,i,n-2i}$ is shown in (5.2) as

$$S(T_{i,i,n-2i}) =$$

$$\begin{vmatrix}
i+(n-2i) & 0 & \cdots & 0 & 1 & \cdots & \cdots & 1 & \cdots\cdots\cdots & 1 \\
0 & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdots\cdots\cdots & \vdots \\
\vdots & \ddots & i+(n-2i) & 0 & \vdots & \vdots & \vdots & \vdots & \cdots\cdots\cdots & \vdots \\
0 & \cdots & 0 & i+(n-2i) & 1 & \cdots & 1 & 1 & \cdots\cdots\cdots & 1 \\
1 & \cdots & \cdots & 1 & i+(n-2i) & 0 & \cdots & 0 & 1 \cdots\cdots & 1 \\
\vdots & \vdots & \vdots & \vdots & 0 & \ddots & \ddots & \vdots & \vdots \cdots\cdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & i+(n-2i) & 0 & \vdots \cdots\cdots & \vdots \\
1 & \cdots & \cdots & 1 & 0 & \cdots & 0 & i+(n-2i) & 1 \cdots\cdots & 1 \\
1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 1 & 2i \;\; 0 \cdots & 0 \\
\vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \vdots & 0 \;\; \ddots \;\; \ddots & \vdots \\
\vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \vdots & \vdots \;\; \ddots \;\; 2i & \vdots \\
1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 1 & 0 \cdots 0 \;\; 2i
\end{vmatrix}. \quad (5.2)$$

Then, to compute the characteristic polynomial of (5.2), we have:

$$\begin{aligned} CH(\mathcal{S}, T_{i,i,n-2i}) &= |\delta I - \mathcal{S}| \\ &= a_0\delta^2 + (a_1 - ((n-2i) + (n-i)^{2i-2} \\ &\quad +(2i)^{(n-2i)-1}))\delta + z_3 \end{aligned} \quad (5.3)$$

and the roots of the equation (5.3) are obtained by solving $|\delta I - \mathcal{S}| = 0$, which resulted in

$$\begin{aligned} &(\delta - (n-2i)(\delta - (n-i)^{2i-2})(\delta - (2i^{(n-2i)-1}) \\ &(a_0\delta^2 + (a_1 - ((n-2i) + (n-i)^{2i-2} + (2i)^{(n-2i)-1}))\delta + z_3) = 0 \end{aligned} \quad (5.4)$$

where $a_0 = 1$ and z_3 is calculated recursively as follows

$$z_1 = \frac{\det \mathcal{S}(T_{i,i,n-2i})}{n-2i}, \qquad where \qquad \det \mathcal{S}(T_{i,i,n-2i}) = a_n \quad (5.5)$$

$$z_2 = \frac{z_1}{n - i^{2i-2}}, \qquad and\ if \quad 2i-2=0 \quad then\ z_2 = z_1 \quad (5.6)$$

$$z_3 = \frac{z_2}{2i^{(n-2i)-1}}, \qquad and\ if \quad (n-2i)-1=0 \quad then\ z_3 = z_2 \quad (5.7)$$

Then, the eigenvalues of $T_{i,i,n-2i}$ given as

$$\begin{aligned} &\delta_2 = n-2i, \delta_3 = (n-i)^{(2i-2)} \ and \quad \delta_4 = (2i)^{(n-2i)-1}. \\ &Then \quad \delta_1 = \frac{B+C}{2} \ and \quad \delta_n = \frac{B-C}{2}, \\ &where \quad B = (a_1) - (\delta_2 + \delta_3 + \delta_4), \quad C = \sqrt{B^2 - 4z_3}. \\ &and \quad a_1 = (2i^2 + 2i(n-2i)) + (2i(n-2i)). \end{aligned} \quad (5.8)$$

□

Some properties of $T_{i,i,n-2i}$ based on $\mathcal{S}(T_{i,i,n-2i})$ can be listed as follows:

- $\delta_n > 0$,
- $\delta_i(T_{2,2,n-4}) > \delta_i(T_{2,2,n-4})$ where $i = 1, 2, 3, \ldots, n$,
- $\delta_n(T_{2,2,n-4}) > \delta_n(T_{2,2,n-4})$,
- $\delta_1 > 0$.

For example, some spectrums of $T_{i,i,n-2i}$, for $i = 1, 4, 5$, are shown in Table 3.

i	n	$T_{1,1,n-2}$
1	4	$0.7639, 2, 2, 5.2361$
	5	$0.6277, 2, 2, 3, 6.3723$
	6	$0.5359, 2, 2, 2, 4, 7.4641$
	7	$0.4689, 2, 2, 2, 2, 5, 8.5311$
i	n	$T_{4,4,n-8}$
4	9	$1, 5^6, 5.6277, 11.3723$
	10	$2, 8, 6^6, 4.8769, 13.1231$
	11	$3, 7^6, 8^2, 4.3765, 11.3723$
	12	$4, 8^3, 8^6, 11.3723$
i	n	$T_{5,5,n-10}$
5	11	$1, 6^8, 7.2984, 13.7016$
	12	$2, 7^8, 10, 6.4174, 15.5826$
	13	$3, 8^8, 10^2, 5.8211, 17.1789$
	16	$6, 10^5, 11^8, 4.6934, 21.3065$

Table 3: The spectrum of $T_{1,1,n-2}$, $T_{4,4,n-8}$ and $T_{5,5,n-10}$ based on $\mathcal{S}(T_{i,i,n-2i})$

6. Extreme Eigenvalues

In this section, the extreme eigenvalues of the connected irregular complete tripartite graph $T_{i,i,n-2i}$ are discussed. A general formula that used to bind the eigenvalue of the graph based on $A(T_{i,i,n-2i})$ is also presented. The comparison with two known formulae Stevanovic [13] and Zhang [14] indicated an improvement upon them.

6.1. Largest eigenvalue based on adjacency matrix $A(T_{i,i,n-2i})$

Let $T_{i,i,n-2i}$ be a complete tripartite graph with n vertices and E edges. Given that A is symmetric then all eigenvalues of $T_{i,i,n-2i}$ are real. Moreover, they are related as follows: $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The spectral radius of $T_{i,i,n-2i}$ that represents the largest eigenvalue is denoted by λ_1. A graph is called regular if $d(v_i) = \triangle$ for all v_i for $i = 1, 2, \cdots, n$. The spectral radius λ_1 of a regular graph is denoted by $\triangle$ [15]. If $x = (x_1, x_2, \cdots, x_n)'$ is the positive eigenvector of $\mathcal{A}(T_{i,i,n-2i})$ corresponding to λ_1, then x is the maximal eigenvector of $T_{i,i,n-2i}$. In the fields of

numerical analysis and social network [14,18], obtaining an estimation of the ratio of components of the maximal eigenvector of G is important. The problem is to estimate the ratio

$$\gamma = \max_{1\leqslant i,j\leqslant n} \frac{x_i}{x_j}.$$

Stevanovic [13] recently studied the spectral radius of connected irregular graphs with n vertices and $\triangle$ maximum degree. In his study, he studied the maximum spectral radius among all of the connected irregular graphs with n vertices and $\triangle$ maximum degree. He showed that

$$\vartheta < \triangle - \frac{1}{2n(n\triangle - 1)\triangle^2} \sim \triangle - \frac{1}{2n^2\triangle^3}. \tag{6.1}$$

Afterward, Zhang [14] improved this formula, and proved that

$$\eta \leq \triangle - \frac{2\triangle - 1 - 2\sqrt{\triangle(\triangle - 1)}}{n(n-1)\triangle)\triangle^2}. \tag{6.2}$$

This bound was later improved by S. M. Cioaba, D. A. Gregory and V. Nikiforov [16], and B. Liu, J. Shen and X. Wang [17].
In this work, we aimed to find the largest eigenvalue λ_1 of $T_{i,i,n-2i}$.

Theorem 6.1. *Let $T_{i,i,n-2i}$ be a simple connected non-regular graph of order n and $|E|$ be the size of $T_{i,i,n-2i}$, with sequence $(d_1, d_2, \cdots, d_n)$. If $X = (x_1, x_2, \cdots, x_n)^T$ is a maximal eigenvector of $T_{i,i,n-2i}$, then*

$$\lambda_1 < \sqrt{\sum_{i=1}^{n} d(v_i)} \quad \textit{where} \quad \sum_{i=1}^{n} d(v_i) = (2i^2 + 4i(n-2i)). \tag{6.3}$$

Proof. From [14], let we recall that

$$\lambda_1 \sum_{i=1}^{n} x_i = \sum_{j=1}^{n} d_j x_j.$$

Let $X = (x_1, x_2, \cdots, x_n)$ be a maximal normalized eigenvector (i.e. $\sum_{i=1}^{n} x_i^2 = 1$) corresponding to λ_1 of $T_{i,i,n-2i}$. Then

$$\left(\lambda_1 \sum_{i=1}^{n} x_i\right)^2 = \left(\sum_{j=1}^{n} d_j x_j\right)^2$$

Firstly let we consider the left hand side of the equation. Since $(x^1, x^2, \cdots, x^n)^T$ is a positive eigenvector of $\mathcal{A}(G)$ corresponding to λ_1 and the value of $\lambda_1 > 0$, then

$$\left(\lambda_1 \sum_{i=1}^{n} x_i\right)^2 \geq \lambda_1^2.$$

Therefore

$$\lambda_1^2 < \left(\sum_{j=1}^{n} d_j x_j \right)^2 .$$

From the right-hand side, we have

$$\left(\sum_{j=1}^{n} d_j x_j \right)^2 \geq \sum_{i=1}^{n} d_i .$$

Hence

$$\lambda_1^2 \leq \sum_{i=1}^{n} d_i$$

then

$$\lambda_1 \leq \sqrt{\sum_{i=1}^{n} d_i}.$$

From 3.1, we have

$$\lambda_1 = \frac{i + \sqrt{i^2 + 4\frac{(2i^2(n-2i))}{i}}}{2} = \frac{i}{2} + \frac{\sqrt{i^2 + 4\frac{(2i^2(n-2i))}{i}}}{2}$$

and

$$\sqrt{\sum_{i=1}^{n} d_i} = \sqrt{(2i^2 + 4i(n-2i))} \geq \sqrt{(2i^2)} + \sqrt{4i(n-2i))}.$$

Comparing with λ_1, we have

$$\frac{i}{2} \leq \sqrt{(2i^2)}$$

and

$$\frac{\sqrt{i^2 + 4\frac{(2i^2(n-2i))}{i}}}{2} \leq \sqrt{4i(n-2i))},$$

then

$$\lambda_1 \leq \sqrt{\sum_{i=1}^{n} d_i}.$$

□

This comparison is shown in Table 5 and Figure 3.

N	$T_{4,4,1}$	$T_{4,4,2}$	$T_{4,4,3}$	$T_{4,4,4}$	$T_{4,4,20}$	$T_{4,4,25}$	$T_{4,4,30}$	$T_{4,4,40}$
Original	5.4641	6.4721	7.2915	8	14.8062	16.2829	17.6205	20
Stevanovic	7.999	7.999	7.999	7.999	23.999	28.999	34	44
Zhang	7.999	7.999	7.999	7.999	23.999	28.999	34	43.999
$\sqrt{\sum_{i=1}^{n} d(v_i)}$	6.9282	8	8.9442	9.7979	18.761	20.784	22.6274	25.9229

Table 4: The spectrum of $T_{4,4,n-8}$

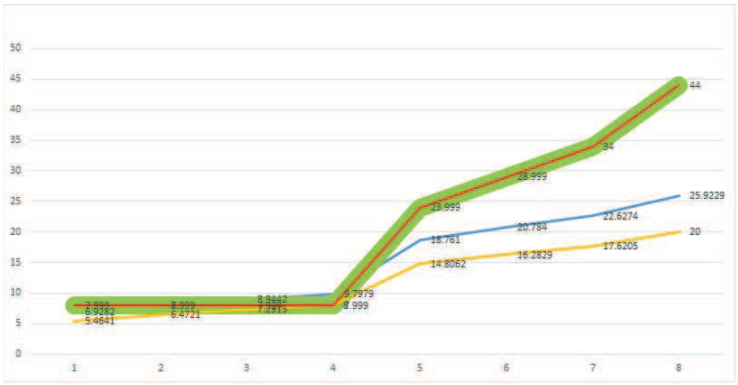


Figure 3: The comparison between Stevanovic, Zhang and the formula (4.4)

7. Chemical Applications of Graph Theory

One of the main applications of the graph spectra is chemistry. The problem encountered in chemical graph theory many years ago was about the existence of molecule graphs with identical spectra. The mathematical properties of the total π-electron energy (E) have a long history as one of the most useful quantum chemical characteristics of a conjugated molecule. This characteristic can be obtained by the theory of unsaturated conjugated hydrocarbons known as the Huckel Molecular Orbital (HMO) theory. The correspondence between the theoretical terms of the graph and the molecular orbital of chemical (chemistry term) is given as follows; in which the vertices correspond to atoms while the edges represent the bound. Huckel matrix [1] is the "adjacency matrix", the graph is the structural formula and a tree graph is the cyclic graph, wherein the degree of the vertices degree is the valence of an atom and the characteristic polynomial is the secular polynomial. This is shown in Table 5.

Chemistry term	Graph theoretical term
Atom	Vertex
Bound	Edge
Acyclic graph	Tree graph
Valence of an atom	Degree of a vertex

n- polygene	Path on a vertex
Secular polynomial	Characteristic polynomial
Huckel matrix	Adjacency matrix
Energy level	Eigenvalue
Bonding level	Positive eigenvalue

Table 5: The chemical term corresponding to the graph theoretical term

Figure [4] represents an example that describes the chemical formula of benzene and its corresponding representation in the graph theory

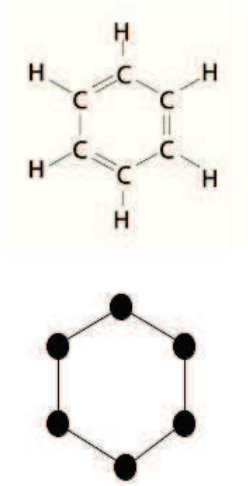


Figure 4: Benzene and its corresponding representation in the graph theory

7.1. Tripartite Energy

Spectral graph theory plays an important role in the molecular orbits of some chemical compounds. In 1930, the German scholar Erich Huckel [1] introduced a method to find the approximation of the solutions of the Schrodinger equation, which refers to a molecular orbital called unsaturated conjugated hydrocarbons. The details of this approach are often referred to as HMO theory. HMO theory is based on the molecular orbital of π-electrons (assuming that the underlying molecule is planar and that the π- and σ-orbitals are mutually orthogonal). The general approximation solution of the HMO model is as follows:

$$H = \alpha I + \beta A(G) \tag{7.1}$$

where H is the Hamiltonian matrix, I is the unit matrix of order n, and $A(G)$ is the adjacency matrix of the corresponding n vertices of the molecular graph. Recall

that, n is the number of conjugated centers in the underlying molecule and that the molecular graph may either be simple (for hydrocarbons) or weighted (for hetero-conjugated systems). The parameters α and β are called the Coulomb and the resonance integrals, respectively. They are regarded as semi-empirical constants. The HMO molecular orbital corresponds to the eigenvectors of the adjacency matrix A. The corresponding energy level is given by

$$E_\pi = \alpha + \beta\lambda_i, \quad i = 1, 2, \cdots, n \tag{7.2}$$

where λ_i is the eigenvalues of A.
In the HMO molecular orbital methods, the total π-electrons are given by

$$E_\pi = \sum_{i=1}^{n} g_i\lambda_i \tag{7.3}$$

where g_i is the "occupation number". We refer to [1] for additional details on this matter. In 1970, Gutman [1] uncovered a relation to determine the total π-electron energy from the molecular orbital of Huckel with the graph theory defined as

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{7.4}$$

The molecular orbital of benzene and hydrocarbon are shown in Figure 5.

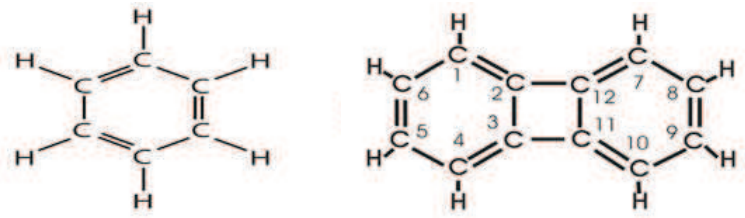


Figure 5: Molecular orbital of benzene C_6H_6 and hydrocarbon $C_{12}H_8$

To represent these two chemical components by the graph theory, the benzene and the hydrocarbon graphs are the tripartite graphs $T_{2,2,2}$ and $T_{4,4,4}$ respectively, such that each carbon atom corresponds to a vertex of the tripartite graph, as shown in Figure [6].

Figure 6: The tripartite graphs $T_{2,2,2}$ and $T_{4,4,4}$

The total $\pi-$ electronic energy of benzene is 8. This value can also be calculated by equation (28) where λ_i for the tripartite graph $T_{2,2,2}$ corresponds to such molecular component.

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| = |-2| + |2| + 4|1| = 8$$

The number of the molecular orbital is symmetric to the tripartite graph $T_{s,t,t}$ where $s = (\frac{n-2}{4})$ and $t = \frac{n-s}{2}$ given as **Naphthalene** $C_{10}H_8$, **Anthracene** $C_{14}H_{10}$, **Tetracene** $C_{18}H_{12}$, **Pentacene** $C_{22}H_{14}$ and in general $C_nH_{(n-2m)}$, where n is the number of carbon atom and $m = ((\frac{n-2}{4})-1)$ is the number of carbon bounds as shown in Figure 7.

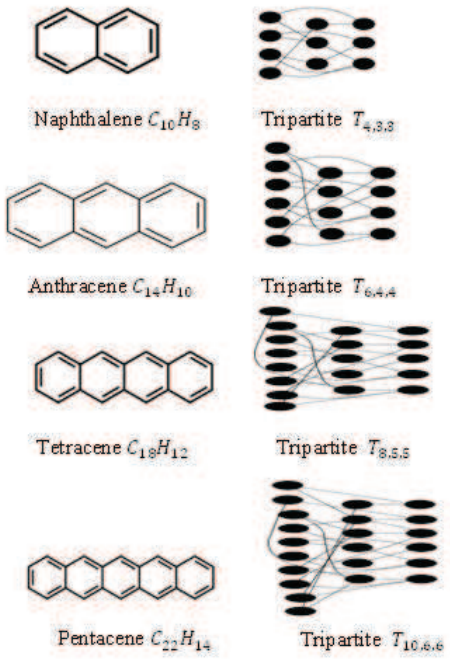


Figure 7: The tripartite graphs corresponding to some molecular orbital.

Therefore, the total $\pi-$electron energy of the molecular orbital of those graphs equals to the summation of the absolute eigenvalues of their corresponding tripartite graphs.
All of the above results are obtained by using the adjacency matrix. The combinatorial Laplacian and signless Laplacian matrices with immense invested interest in chemistry are presented for future works.
In 2006, Gutman and Zhou [19] defined the energy of the graph called Laplacian

energy of G denoted by LEG, and given as:

$$LEG = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n}| \tag{7.5}$$

where $\mu_i (i = 1, \cdots, n)$ are the eigenvalues of the Laplacian matrix L obtained by using (7.5), and m, n are the numbers of edges and vertices of G, respectively. Several properties are known especially to bind the energy and the Laplacian energy of a graph. For example, the total π-electron energy of benzene is given by:

$$LEG = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n}| = |0 - \frac{12}{6}| + 2|1 - \frac{12}{6}| + 2|3 - \frac{12}{6}| + |4 - \frac{12}{6}| = 8$$

For more details about the Laplacian energy of a graph based on the signless matrix, we refer the reader to see [20,21].
Some total π-electron energy of molecular orbital of hydrocarbon $C_nH_{(n-2((\frac{n-2}{4})-1))}$, can be found by the eigenvalues of the tripartite graph $T_{s,t,t}$, as shown in Figure 8.

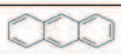
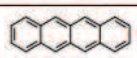
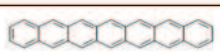
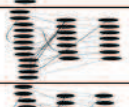
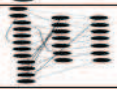
Name	Formula $C_nH_{n-2((\frac{n-2}{4})-1)}$	Molecular orbital of $C_nH_{n-2((\frac{n-2}{4})-1)}$	Tripartite graph $T_{s,t,t}$	Total π-electron energy
Benzene	C_6H_6			8
Naphthalene	$C_{10}H_8$			13.68
Anthracene	$C_{14}H_{10}$			19.3136
Tetracene	$C_{18}H_{12}$			24.3515
Pentacene	$C_{22}H_{14}$			30.54
Hexacene	$C_{26}H_{16}$			36.0297
Heptacene	$C_{30}H_{18}$			40.7311
Octacene	$C_{34}H_{20}$			46.3532

Figure 8: Some types of $C_nH_{(n-2((\frac{n-2}{4})-1))}$ with the structures of their corresponding tripartite graph

We found that the total π-electron energy for **benzene**, **hydrocarbon**, **Naphthalene**, and **Anthracene** equal to the sum of the eigenvalues of their corresponding tripartite graphs $T_{s,s,t}$ based on the adjacency matrix.

8. Conclusions

This paper focused on the important subject in mathematics called the spectral graph theory which combines the graph theory and linear algebra. New results of the spectral graphs was studied. Main concern was for the tripartite graph. The obtained theoretical results can be compared with the practical results to prove their validity. The spectrum of some graphs based on adjacency matrix and Laplacian matrix (combinatorial and signless) was studied, especially, for the complete tripartite graphs $T_{(i,i,n-2i)}$. The extreme eigenvalues (maximum and minimum eigenvalues) were the main achievement in this work. The general formula of the largest eigenvalue of tripartite graph $T_{(i,i,n-2i)}$ was presented depending on the properties of the graph. A new formula for extreme eigenvalues of some connected irregular complete tripartite graph was proposed and showed an improvement upon some well-known methods in this field. Satisfactory results were obtained upon applying these new methods in quantum chemistry. We found that, the molecular orbital of some chemical compounds, such as hydrocarbon $C_nH_{(n-2m)}$ and unit cell of crystal, could be represented by the tripartite graph because they had the same structure. Also, the total π- electronic energy levels for those chemical compounds could be calculated by summing the absolute values of the spectrum of their corresponding graphs.

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Nawras A. Alawn,
Department of applied Sciences,
University of Technology,
Baghdad, Iraq.
E-mail address: nawrasalwan@gmail.com

and

Nadia M.G. Al-Saidi, Department of applied Sciences,
University of Technology,
Baghdad, Iraq.
E-mail address: nadiamg08@gmail.com

and

Rashed T. Rasheed,
Department of applied Sciences,
University of Technology,
Baghdad, Iraq.
E-mail address: r_awsy@yahoo.com