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Cite as: AIP Conference Proceedings **2086**, 030006 (2019); https://doi.org/10.1063/1.5095091
Published Online: 02 April 2019

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

The Energy of a Tripartite Graph

Nawras A. Alawn[1,a)], Nadia M.G. Al-Saidi and Rashed T. Rasheed

[1]*Department of Applied Sciences, University of Technology, Baghdad, Iraq*

[a)]Corresponding author: nawrasalwan@gmail.com

Abstract. The energy of a graph is used to approximate the total π-electron energy of molecules. Thus, finding a new technique that facilitates this task is a challenge that has received increased research attention. This paper introduces the eigenvalues of a complete tripartite graph $T_{i,i,n-2i}$, for $n \geq 4$, with respect to the adjacency, Laplacian, and signless Laplacian matrices. The chemical HMO approach is particularly successful in the case of the total π-electron energy. Experiments reveal that some chemical components are equienergetic with the tripartite graph. This finding helps easily derive the HMO of most of these components despite their different structures.

Keywords: Tripartite graph, Adjacency matrix, Laplacian matrix, Signless matrix , Characteristic polynomial.
2010 Mathematics Subject Classification: 68R10, 81Q30, 97K30.

INTRODUCTION

Spectral graph theory emerged in the 50s. Apart from graph theoretical research on the relationship between the structural and spectral properties of graphs, another major research was sourced in quantum chemistry. The connections between these two lines 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 to date. This summary was updated by a survey of the recent theory of graph spectral results.

Spectrum has several applications in chemical, physics, medicine, computer science, information theory, geographic studies, and social sciences among others. 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 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 has also been applied in medical sciences, including in 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].

The adjacency matrix $\mathcal{A}(G)$ is define by 0, 1, whose (i, j) entry is 1 if $(v_i, v_j) \in E$, and 0 otherwise [13]. 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 of all vertices degrees called degree matrix. 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 Laplcain 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 $T_{i,i,n-2i}$ [14] 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 play 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].

International Conference of Mathematical Sciences (ICMS 2018)
AIP Conf. Proc. 2086, 030006-1–030006-4; https://doi.org/10.1063/1.5095091
Published by AIP Publishing. 978-0-7354-1816-5/$30.00

In this article, the spectrum of this graph is discussed, and general formulas are construed based on adjacency, Laplacian, and signless Laplacian matrices. The extreme eigenvalues (maximum and minimum eigenvalues) are also demonstrated. In 2004, Stevanovic [9] 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 [9] and Zhang [10] formula.

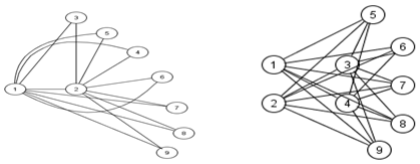

FIGURE 1. Complete tripartite graphs $T_{1,1,7}$,$T_{2,2,5}$

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 $\mathcal{A}$.

Theorem 0.1 *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 $\mathcal{A}$ are:*

$$\{0^3, -i, \frac{i+\sqrt{i^2+4g}}{2}, \frac{i-\sqrt{i^2+4g}}{2}\} \tag{1}$$

THE EIGENVALUES OF $T_{I,I,N-2I}$ BASED ON LAPLACIAN MATRIX $\mathcal{A}$

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

Theorem 0.2 *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 general formula of eigenvalues of $T_{i,i,n-2i}$ based on Laplacian matrix L are:*

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

THE EIGENVALUES OF $T_{I,I,N-2I}$ BASED ON SIGGNLESS LAPLACIAN MATRIX $\mathcal{A}$

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

Theorem 0.3 *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 are:*

$$\{n-2i, (n-i)^{(2i-2)}, (2i)^{(n-2i)-1}, \frac{B+C}{2}, \frac{B-C}{2}\} \tag{3}$$

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

CHEMICAL APPLICATIONS OF GRAPH THEORY

One of the main applications of graph spectra is chemistry. The problem encountered in chemical graph theory many years ago is 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 graph theoretical terms and the molecular orbital of chemical (chemistry term) given as follows, where the vertex is the atom, edge is the bound, Huckel matrix [1] is the "adjacency matrix", graph is the structure formula, and a tree graph is the cyclic graph, wherein the vertices degree is the valence of an atom and the characteristic polynomial is the secular polynomial.

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 approximate Schrodinger equation solutions, which refers to a molecule orbital called unsaturated conjugated hydrocarbons. The details of this approach are often referred to as HMO theory. HMO theory is based on the molecule 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:

$$H = \alpha I + \beta A(G) \tag{4}$$

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 molecular graph. The parameters α and β are called the Coulomb and the resonance integrals, respectively. They are regarded as semi-empirical constants. The HMO molecule orbital corresponds to the eigenvectors of the adjacency matrix A. The corresponding energy levels are:

$$E_\pi = \alpha + \beta\lambda_i, \quad i = 1, 2, \cdots, n \tag{5}$$

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

$$E_\pi = \sum_{i=1}^{n} g_i \lambda_i \tag{6}$$

where g_i is the occupation number. 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 molecule orbital of Huckel with graph theory defined as:

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \tag{7}$$

The molecular orbital of benzene and hydrocarbon are shown in Figure 2.

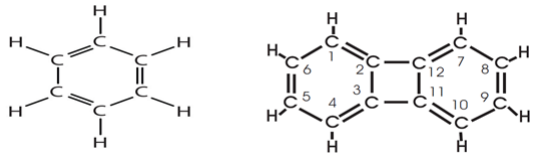

FIGURE 2. Molecular orbit of benzene C_6H_6 and hydrocarbon $C_{12}H_8$

To represent these two chemical components by graph theory, the benzene and 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 3.

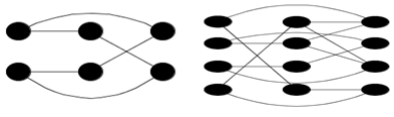

FIGURE 3. The tripartite graphs $T_{2,2,2}$ and $T_{4,4,4}$

Given that the total π electronic energy of benzene is 8, this value can also be calculated by equation (7) where λ_i for the tripartite graph $T_{2,2,2}$ correspond to such molecular component.

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

A number of the molecular orbital are symmetric to the tripartite graph $T_{s,t,t}$ where $s = (\frac{n-2}{4})$ and $t = \frac{n-s}{2}$ are as follows: **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 $m = ((\frac{n-2}{4}) - 1)$ the number of carbon bounds as shown in Figure 4.

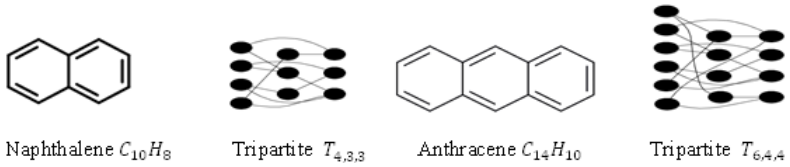

FIGURE 4. The tripartite graphs corresponding to some molecular orbital.

Therefore, the total π-electron energy of the molecular orbital of those graphs equals the summation of the absolute eigenvalues of their corresponding tripartite graphs.
All of the above results are obtained using the adjacency matrix. The combinatorial Laplacian and signless Laplacian matrices with immense invested interest in chemistry are presented for future works.

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