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VAN YÜZÜNCÜ YIL UNIVERSITY
INSTITUTE OF NATURAL AND APPLIED SCIENCES
DEPARTMENT OF MATHEMATICS

ON THE NULLITY OF SOME GRAPHS STRUCTURES

M.Sc. THESIS

PRESENTED BY: Jafar Muhammad TELI
SUPERVISOR: Assist. Prof. Dr. Mehmet Şerif ALDEMİR

VAN - 2017

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ACCEPTANCE and APPROVAL PAGE

This thesis entitled **"ON THE NULLITY OF SOME GRAPHS STRUCTURES"** presented by Jafar Muhammad TELI under supervision of Assist. Prof. Dr. Mehmet Şerif ALDEMİR in the Department of Mathematics, Faculty of Science, Yüzüncü Yıl University has been accepted as a M. Sc. Thesis according to Legislations, of Graduate Higher Education on 18 /08 / 2017 with unanimity of members of jury.

Chair: Assoc. Prof. Dr. Ali SIRMA Signature:

Member: Assist. Prof. Dr. Süleyman EDİZ Signature:

Member: Assist. Prof. Mehmet Şerif ALDEMİR Signature:

This thesis has been approved by the committee of the Institute of Science on ..../......../ 2017 with decision number..................

Signature

....

Director of Institute

THESIS STATEMENTS

All information presented in the thesis was obtain in the frame of according to ethical behavior and academic rules, in addition all kinds of informations that does not belong to me have been cited appropriately in the thesis and this thesis was prepared in the light of the thesis writing rules.

Signature

ABSTRACT

ON THE NULLITY OF SOME GRAPHS STRUCTURES

Jafar Muhammad TELI
M. Sc. Thesis, Mathematics Science
Supervisor: Assist. Prof. Dr. Mehmet Şerif ALDEMİR
August 2017, 42 pages

This master thesis study, which is consists of three chapters, was presented some last studies about the nullity of some simple and chemical graphs. Chapter one consists of literature review, some basic definitions in graph theory and some results and relations between graphs and matrices. Chapter two gave basic definitons of graph nullity, nullity applications of some simple graphs and relations between nullity and some graph structures. Chapter three investigated the relations between nullity of some molecular graphs of chemical compounds and their chemical properties.

Keywords: Chemical graphs, Graph's spectrum, Nullity,

ÖZET

BAZI BASİT GRAFLARIN SIFIRLIĞI

Jafar Muhammad TELI
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Üç bölümden oluşan bu tez çalışmasında bazı özel sonlu ve kimyasal grafların spektrumlarının sıfırlığıyla ilgili yapılan son çalışmalar sunuldu. Birinci bölüm, literatür taramasından, bazı temel graf teorisi tanımlarından ve graflar ve matrisler arasınndaki ilişkilerden oluşmaktadır. İkinci bölüm, graf sıfırlığının temel tanımlarını, bazı basit grafların sıfırlık uygulamalarını ve bazı graf yapılarıyla graf sıfırlığı arasındaki ilişkileri vermektedir. Üçüncü bölümde, bazı kimyasal grafların sıfırlığıyla kimyasal özellikleri arasındaki ilişkileri incelendi.

Anahtar kelimeler: Grafların spektrumu. Kimyasal graf, Sıfırlık,

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Jafar Muhammad TELI

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LIST OF SYMBOLS

Some symbols and abbreviations used in this study are presented below, along with descpriptins.

Symbols	**Explanations**
A(G) or A = [a_{ij}]	Adjacency matrix of G
C_p	Cycle graph with p vertices
Det(A)	Determinant of a matrix A
deg(v)	Degree of the vertex v in G
E(G)	Set of edges of G
G(V, E)	Simple Graph
$G \cong H$	Isomorphic graphs G and H
$G_1 \cup G_2$	Union of graphs G_1 and G_2
$(\mathbf{G_1} \cap \mathbf{G_2})$	The intersection G_1 and G_2
G-v	Deleting a vertex v from G
$\bar{G}$ or G^c	Complement of G
I_p	The identity matrix of order p
K_p	Complete graph with p vertices
$K_{m,n}$	Complete bipartite graph with $m+n$ vertices
L(G)	Line graph of G
B(G)	Matching number of G
N_p	Null graph of order p
p(G)	Number of vertices of G (order of G)
P_p	Path graph with p vertices
q(G)	Number of edges of G (size of G)
r(G)	Rank of the adjacency matrix of G
$S_p(G)$	Spectrum of a graph G

Symbols	**Explanations**
$S_{1,\,p-1}$	Star graph with p vertices
T_p	Tree, Tree with p vertices
V(G)	Set of vertices of G
W_p	Wheel graph with p vertices
$\varphi(G;x)$	Characteristic polynomial of G
η(G)	Nullity of G
$\lfloor \mathbf{x} \rfloor$	the greatest integer of the number x
G^+	A graph G by adding a loop to each of its vertices
N_G(v)	eighborhood of the vertex v in G
Δ(G)	Maximum degree of G
δ(G)	Minimum degree of G
κ(G)	Connectivity of G
$d_G(u,v)$	Distance between two vertices u and v in G

1. INTRODUCTION

Graph theory is a branch of mathematics which studies the structure of graphs and net works, in the domain of mathematics and computer science, graph theory is the study of graphs that concerns with the relationship among edges and vertices. It is a popular subject having its applications in computer science, information technology, bioscience, mathematics, and linguistics to name a few, graph theorical concepts are widely used to study and model various applications in different areas, they include study of molecules constraction of bonds in chemistry and the study of atoms.

Graph theory has become an important for its applications in computer science, communication Networks. It has seen increasing interactions with other areas of mathematics, (Seehu, 1961).

There are several objects which are nowadays naturally described as graphs. A graph is an ordered pair of a non-empty set of objects called "vertices" together with a set of unordered pairs of distinct vertices called "edges" (Ruohonen, 2013).

In this thesis, we consider finite connected undirected graphs without loops and multiple edges, with labeled vertices and some properties of nullity of some simple graphs that was studied by (Ali et al., 2016a; Sharaf and Rasul, 2014), they proved that if G is a graph containing a vertex of degree one and H be the sub graph obtained from G, by deleting this vertex together with the vertex adjacent to it, then $\eta(G) = \eta(H)$. This procedure is named as "End Vertex Corollary". (Sharaf and Rasul, 2014).

And we go to explain how chemical molecule can be represented by a graphs and the role of the nullity in chemistry for some molecular graphs, by taking atoms of different molecule as a vertex connected by atomic bounds making the edges of a graph. The nullity of a (molecular) graph G, denoted by $\eta(G)$, is the algebraic multiplicity of the number zero in the spectrum of the adjacency matrix of the (molecular) graph (Balakrishnan and Ranganathan, 2012; Bonchev, 2013).

The different structural of same chemical fomula haveing same properties are called isomers, isomers are two nonisomorphic graphs having the same degree sequence (Bocker et all, 2011; Balakrishnan and Ranganathan, 2012).

The characteristic polynomial of graph G, is the characteristic polynomial of its adjacency matrix A(G) , denoted by $\varphi(G;x)$. Since A(G) is a real symmetric matrix, its eigenvalues are real numbers.

when A(G) is a singular matrix A graph G is said to be singular, the eigenvalues of the graph G, is the eigenvalues λ_1, λ_2, ..., λ_p of A(G) and form the spectrum of this graph, the occurrence of zero as an eigenvalue in the spectrum of the graph G is called the "nullity" denoted by η(G). It represents the stability in chemical compound graphs (Ali et al 2016a), (Gutman and Bojana 2009); (Sharaf and Rasul, 2014).

In this thesis, we continue the research along the same lines. We derive formulas to determine the nullity of molecule of chemical compound graphs. And we go to explain the role of the nullity in chemistry and nullity of some molecular graphs. For some chemical compounds graphs.

This master thesis consists of 3 chapters. Chapter 1 is introductions consists the general background notions, and important definition on graph theory, and relations between graphs and matrices.

Chapter 2, nullity of graph and the degree of singularity of graphs, by solving the characteristic polynomial of a graph.

Chapter 3, we study the nullity of chemical formula graphs and some applications on graph spectra and the relation between degree of singularity and the instability of the molecule graph of chemical compounds.

Finally, the last section covers conclusion which winds up the result of this study.

1.1 General Background in Graph Theory

This section presents some basic definitions, terminologies and notions in graph theory, along with fundamental results. Further information can be found in the standard books: (Balakrishnan and Ranganathan, 2012; Chartrand and Zhang, 2012; Bondy and Murty, 1982; Balakrishnan and Ranganathan, 2012; Ruohonen, 2013; Voloshin 2009; Zaidan, 2003; Bienke and Wilson, 2005;).

1.2. Graph Theory Fundamentals

A graph is a diagram of points and lines connected to the points, it has at least one line joining of two vertices with no vertex connecting itself, the concept of graphs in graph theory stands up on some basic terms such as point, line, vertex, edge, degree of vertices, properties of graphs, graph theory started with the problem of Konigsberg Bridge in 1736 by Euler when he want to solve the Konigsberg Bridge problem that lead to the concept of Eulerian graphs (Seshu, 1961).

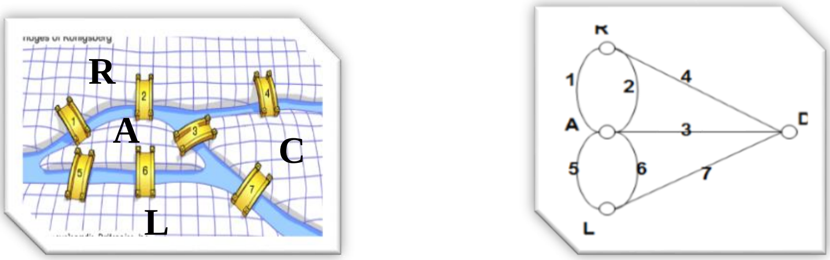


Figure 1.1. Konigsberg Bridges.

A point can be denoted by an alphabet, it can be represented with a dot, a line is a connection between two points, it can be represented with a solid line, a vertex is a point where multiple lines meet, it is also called a node, similar to points, a vertex is also denoted by an alphabet, an edge is the mathematical term for a line that connects two vertices, many edges can be formed from a single vertex, without a vertex an edge cannot be formed, there must be a starting vertex and an ending vertex for an edge, graphs come with various properties which are used for characterization of graphs depending on their structures, these properties are defined in specific terms pertaining to the domain of graph theory (Tutuorials Point, 2014). ***www.tutuorialspoint.com.***

1.3. Some Basic Definitions

Definition1.1. A graph is an order pair G = (V, E), where V is a nonempty set of vertices, E is the set of edges (disjoined from V) connecting the pairs of vertices, a graph is finite if its vertex set and edge set are finite (Zaidan 2003; Voloshin 2009; Wilson, 2010; Balakrishnan and Ranganathan, 2012; Ruohonen, 2013).

The number of vertices p in a graph is the order of the graph, the number of edges q is the size of the graph . a graph with only one vertex is trivial graph, and when q=0, a graph of zero size is an empty (null) graph. A null graph with p vertices is denoted by N_p .

Graph G is labeled graph when the p vertices are labeled by names such as v_1, v_2, …, v_p, the edge written as uv, mean that edge joins u and v and it is incident u with v, that u and v are adjacent vertices, or neighbors N(v).

Degree of a vertex v, deg(v), is the number of neighbors, sum of the degrees of vertices in a graph is twice the number of its edges.

G is regular graph If all the degrees of vertex of G are equal, zero degree vertex is called an isolated vertex, end vertex is the vertex of degree one. the degrees sequence of the vertices of G, is degree sequence D_G, of G.

A walk in a graph G is vertices and edges sequence v_0, e_1, v_1, …, e_k, v_k, the length of the walk is number of edges, closed walk if started and finished vertex are the same, and is open if started and finished vertex are differente.

If all vertices of walk are distinct walk is a path, if all edges are distinct walk is a trail, a walk is cycle when it is closed that its k vertices are distinct and $k \geq 3$, the number of edges between two vertex u and v is the distance between u and v.

H is a subgraph of a graph G when all vertices and edges of H are in G. If order of H equales order of G, then H is a spanning subgraph.

If each pair of vertices of G are connected by path then a graph G is connected, opposite of that it is disconnected, a maximal connected subgraph of G is a component of G.

A path graph P_n is a graph whose vertices can be arranged by v_1, v_2,..,v_n, in which v_i is adjacent with v_{i+1} for i = 0 to n – 1, the cycle graph C_n is a path with an edge joining v_1 to v_n. The complete graph K_n is a graph with n vertices in which an two vertices are adjacent.

The complete bipartite graph $K_{m,n}$, is a graph with two bipartite sets of vertices, say v_1 order v_1 = m, and v_2 order v_2 = n, in which every vertex of v_1 is a adjacent with every vertex of v_2.

The complement $G^c$of a graph G is a graph whose vertices are vertices of G and two vertices u and v are adjacent in G^c, if u and v are non-adjacent in G.

Awheel graph W_p. for $p \geq 4$, of order p consisting of a cycle C_{p-1} together with a vertex adjacent to every vertex of C_{p-1}.

A graph with one cycle is un-icycle graph, if a graph G has no cycles called acyclic, a connected acyclic graph is called a tree, and is denoted by T_p.

Star graph $K_{m,n}$, is a star graph when m consists of exactly one vertex and it is denoted by $S_{1,n}$ or S_n.

A graph can exist in different forms having the same number of vertices, edges and also the same edge connectivity, such graphs are called isomorphic graphs, graph G_1 , G_2 are said to be isomorphic(have the same structure), write $G_1 \cong G_2$, if order of G_1 equals order G_2, size of G_1 equals size of G_2, and degree squences of G_1 and G_2 are same, there exists a bijection fuction f : V (G_1) → V (G_2),from vertices of G_1 to vertices of G_2 , without bijection fuction f: V (G_1) → V (G_2), the graph G_1 and G_2 are non-isomorphic graph, and a graph is planer if it can be drawn without crossing edges.

Definition 1.2. The join $G_1 + G_2$ of two graphs G_1 and G_2 is a graph whose vertex set is $V(G_1+G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1+G_2) = E(G_1) \cup E(G_2) \cup \{u\,v: \forall\, u \in G_1$ and $\forall\, v \in G_2\}$ (Sharaf and Rasul 2014).

Definition 1.3. A matching M is the independent edges subset set of a graph G if no two edges of M are adjacent in G, (a set of independent edges), and maximum M is called the matching number of G, denoted by B(G) (Balakrishnan and Ranganathan, 2012).

The maximum numbers of edges possible is, $\frac{n(n-1)}{2}$, n is order of a graph.

The numbers of simple graphs possible is, $2^{\frac{n(n-1)}{2}}$

If $n = 3$ we have $\frac{3(3-1)}{2} = \frac{6}{2} = 3$ edges

$\frac{3(3-1)}{2} = \frac{6}{2} = 3^2 = 8$ simple graphs .

1.4. Matrices Representation of Graphs

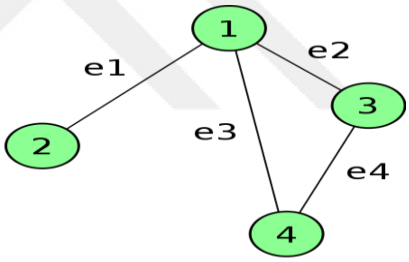
Is the way to represent undirected and directed graphs in the form of matrix by Adjacency matrix represents adjacent vertices and incidence matrix represents vertex-edge incidences. Matrix representations provide a bridge to linear algebra (Zaidan, 2003; Ruohonen, 2013;).

Definition 1.4. The adjacency matrix of the labled simple finit graph G = (V, E) is an n x n matrix D = (d_{ij}), where n is the number of vertices in G, V = $\{v_1, v_2, \ldots, v_n\}$ and d_{ij} = number of edges between v_i and v_j. In particular d_{ij} = 0, if (v_i, v_j) is not an edge in G (Ruohonen, 2013).

1.5. Properties of Adjacency Matrix

- The interior along the principal diagonal of A are all 0 if and only if the graph has no self – loop , a self – loop at the k_{th} vertex corresponds to a_{kk}=1
- The adjacency matrix A is symmetric without parallel edges.
- if the graph has no self-loops, the degree of a vertex equals the number sum of one in the corresponding row or column of A.
- therefore an isolated vertex is represented by a row with all zeros (Ruohonen, 2013).

$$D = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$



$$A = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{bmatrix}$$

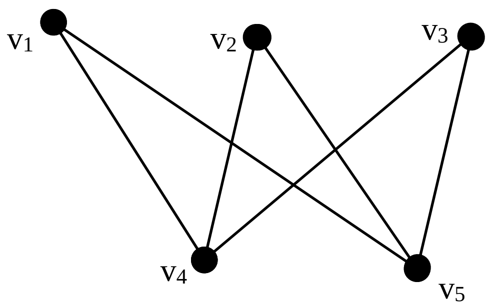


Figure1.2. Adjacency Matrix of graphs.

1.6. Representation of Trees:

Tree is a connected graph without cycles, a graph without cycles is called un-acyclic graph or a forest, so each component of a forest is a tree, (Balakrishnan and Ranganathan, 2012).

$$
T = \begin{matrix} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \end{matrix}
\begin{bmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 \\
0 & 1 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0
\end{bmatrix}
$$

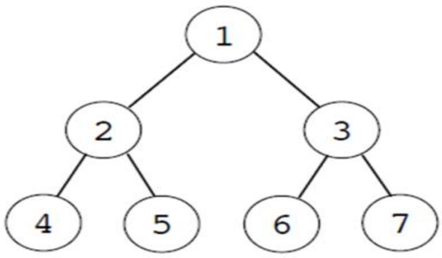


Figure1.3. Representation of Tree.

1.7. Eulerian Graphs: An Eulerian graph is a connected graph that has a closed trial containing every edge only once (every vertex must have even degrees), an Eulers path contains of each edge of graph exactly once (started and finished in different vertex), in an Eulers path if the starting vertex is the same as its ending vertex(started and ended in the same vertex), then it is called an Eulers circuit. (Balakrishnan and Ranganathan, 2012).

Figure1.4. Eulerian Graph.

2. NULLITY OF GRAPHS

Nullity of graph, immediately three numbers come in the mind, first is order, second is size and third is the components k of graph, that important to know rank and nullity (Sharaf and Rasul, 2014).

2.1. Null Space

If A is an ($m \times n$) matrix, null space of A is the solution space of the linear system Ax=0, which is a subspace of R^n .

A graph G is singular of nullity η if the null space of its adjacency matrix A has dimension n. Such that a graph contain n vectors determined by basis for the null space of A (Anton and Rorres, 2010).

Definition 2.1.

The spectra $S_P(G)$ of a graph G is a matrix with two rows, one row is eigenvalues, and two rows are their multiplicity (Balakrishnan and Ranganathan, 2012).

That if we have an eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ with multiplicities $m(\lambda_1), m(\lambda_2), \ldots, m(\lambda_n)$ respectively, then we write, (Sharaf and Rasul, 2014).

$$sp(G) = \begin{bmatrix} \lambda_1 & \lambda_2 & . & . & \lambda_n \\ m_1 & m_2 & . & . & m_n \end{bmatrix}$$

Example: the nullity of identity matrix (I) is zero, but rank of $I_{n \times n}$ is equal to n.

$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$, identity matrix r(A)= 3, η(A) = 0

$$Q(I_4\,, x) = |xI - A| = \left| x\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \right| = \begin{vmatrix} x-1 & 0 & 0 & 0 \\ 0 & x-1 & 0 & 0 \\ 0 & 0 & x-1 & 0 \\ 0 & 0 & 0 & x-1 \end{vmatrix}$$

$$= x - 1 \begin{vmatrix} x-1 & 0 & 0 \\ 0 & x-1 & 0 \\ 0 & 0 & x-1 \end{vmatrix} = (x-1)^4$$

$$(x-1)^4 = 0, that, x = 1, four\ times, s_p(I_4) = \begin{bmatrix} 1 \\ 4 \end{bmatrix}$$

For some classes, of graphs the spectrum is known and its nullity η.

Lemma 2.2. (Sharaf and Rasul, 2014).The nullity of the wheel graph W_n , is:

$$\eta(W_n)=\begin{cases} 2, & if\ n\equiv 1(\mathrm{mod}4), \\ 0, & otherwise. \end{cases}$$

Lemma 2.3. (Sharaf and Rasul, 2014).

i) The nullity of the cycle graph C_n , is:

$$\eta(C_n)=\begin{cases} 2, & if\ n\equiv 0(\mathrm{mod}4), \\ 0, & otherwise. \end{cases}$$

ii) The nullity of the path graph P_n , is:

$$\eta(P_n)=\begin{cases} 1, & if\ n\ is\ odd, \\ 0, & if\ n\ is\ even. \end{cases}$$

iii) The spectrum of the complete graph K_n , is:

$$S_p(K_n)=\begin{pmatrix} n-1 & -1 \\ 1 & n-1 \end{pmatrix}.$$

Thus
$$\eta(K_n)=\begin{cases} 1, & if\ n=1, \\ 0, & if\ n>1. \end{cases}$$

Examples;

$$S_p(K_4)=\begin{pmatrix} 4-1 & -1 \\ 1 & 4-1 \end{pmatrix}$$

$$S_p(K_4)=\begin{pmatrix} 3 & -1 \\ 1 & 3 \end{pmatrix}$$

$$S_p(K_{100})=\begin{pmatrix} 99 & -1 \\ 1 & 99 \end{pmatrix}$$

iv) The spectrum of the complete bipartite graph $K_{m,n}$, is:

$$S_p(K_{m,n})=\begin{pmatrix} \sqrt{mn} & 0 & -\sqrt{mn} \\ 1 & m+n-2 & 1 \end{pmatrix}$$

Thus
$$\eta(K_{m,n})=\begin{cases} 0, & if\ m=n=1, \\ m+n-2, & otherwise. \end{cases}$$

Example;

$$S_p(K_{2,3})=\begin{pmatrix}\sqrt{6} & 0 & -\sqrt{6}\\ 1 & 3 & 1\end{pmatrix}$$

v) The spectrum of the null graph N_n , is:

$$S_p(N_n)=\begin{pmatrix}0\\ n\end{pmatrix} \;,\; S_p(N_{100})=\begin{pmatrix}0\\ 100\end{pmatrix}$$

$$\eta(N_n)=n \quad \eta(N_{100})=100$$

Definition 2.4. A graph G is a singular graph when determinant of A(G)=0, then eigenvalues of A(G) are that of G, which forms the spectrum of G, nullity is the number of zero in the spectrum of G denoted by η(G) (Sharaf and Rasul 2014).

Definition 2.5. If A is n × n matrix represent graph G (with order p) the number λ is defined an eigenvalues of A(G), which satisfy Det (xI_p-A)=0, or λ is an eigenvalues of G if there exist a non-zero p × 1 vectors X such that AX=λX, then X represent eigenvector of A (Anton and Rorres, 2010; Balakrishnan and Ranganathan, 2012).

Null graph is a graph with n vertices without edge denoted by N_n, the adjacency matrix A(N_n), is n x n zero matrix, the set of eigenvalues of N_n is {0,0,0,…,0}, n times, the spectra of null graph, $S_p(N_n) = \begin{bmatrix}0\\ n\end{bmatrix}$, η(N_n)= n, (Sharaf and Ali, 2014).

Example: The nullity of zero matrix $(0)_{m \times n}$ is n, and rank of zero matrix is zero.

$$B = \begin{bmatrix}0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{bmatrix} \;,\; \text{zero matrix } r(B) = 0 \;, \quad \eta(B) = 3$$

$$Q(N_4\,, x) = |xI - A| = \left| x\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix} - \begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}\right| = \begin{vmatrix}x & 0 & 0 & 0\\ 0 & x & 0 & 0\\ 0 & 0 & x & 0\\ 0 & 0 & 0 & x\end{vmatrix}$$

$$= x\begin{vmatrix}x & 0 & 0\\ 0 & x & 0\\ 0 & 0 & x\end{vmatrix} = x^2\begin{vmatrix}x & 0\\ 0 & x\end{vmatrix} = x^4, \qquad x^4 = 0, that, x = 0, four\ times$$

$$S_P(N_4) = \begin{bmatrix}0\\ 4\end{bmatrix}$$

Definition 2.6. The characteristic polynomialof A(G) is the characteristic polynomial of graph G denoted by φ(G; x) = Det (xI_p-A) = $(-1)^p$ Det$(A - xI_p)$,

φ(G; x) with order p is a polynomial of degree p,

That, φ(G; x) = $a_0x^p + a_1x^{p-1} + \ldots + a_{p-1}x + a_p$, (Balakrishnan and Ranganathan, 2012),

$$A(K_4) = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

$$Q(K_4, x) = |xI - A| = \left| x \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix} \right|$$

$$= \begin{vmatrix} x & -1 & -1 & -1 \\ -1 & x & -1 & -1 \\ -1 & -1 & x & -1 \\ -1 & -1 & -1 & x \end{vmatrix} = \begin{vmatrix} x & -1 & -1 & -1 \\ -1-x & x+1 & 0 & 0 \\ -1-x & 0 & x+1 & 0 \\ -1-x & 0 & 0 & x+1 \end{vmatrix}$$

$$R_2 = R_2 - R_1$$

$$R_3 = R_3 - R_1$$

$$R_4 = R_4 - R_1$$

$$C_1 = C_1 + C_2 + C_3 + C_4$$

$$= \begin{vmatrix} x-3 & -1 & -1 & -1 \\ 0 & x+1 & 0 & 0 \\ 0 & 0 & x+1 & 0 \\ 0 & 0 & 0 & x+1 \end{vmatrix} = (x-3) \begin{vmatrix} x+1 & 0 & 0 \\ 0 & x+1 & 0 \\ 0 & 0 & x+1 \end{vmatrix}$$

$$= (x-3)(x+1)^3$$

$$(x-3)(x+1)^3 = 0, \qquad x = 3, \qquad x = -1\,, \textit{three times}$$

$$S_P(K_4) = \begin{bmatrix} n-1 & -1 \\ 1 & n-1 \end{bmatrix}, \quad S_P(K_4) = \begin{bmatrix} 3 & -1 \\ 1 & 3 \end{bmatrix}$$

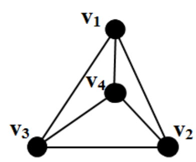


Figure 2.1. complete graph K_4.

Theorem 2.7. The number of vectors that form the basis for the solution space of A, is called nullity of A (Anton and Rorres, 2010).

A general system of linear equations can be written as:

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b1$$

$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b2 \quad \ldots\ldots\ldots\ldots\ldots\ldots.. \quad (1)$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

$$a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n = bn$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & --- & a_{1n} \\ a_{21} & a_{22} & a_{23} & --- & a_{2n} \\ a_{31} & a_{32} & a_{33} & --- & a_{3n} \\ . & . & . & . & . \\ . & . & . & . & . \\ a_{m1} & a_{m2} & a_{m3} & --- & a_{mn} \end{bmatrix} * \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ . \\ . \\ x_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ . \\ 0 \\ 0 \end{bmatrix} \quad \ldots\ldots\ldots\ldots. \quad (2)$$

To find basis null space from matrix A, we find Echelon form (Anton and Rorres, 2010).

$$A = \begin{bmatrix} 1 & 3 & 0 & 2 & 6 & 3 & 1 \\ -2 & -6 & 0 & -2 & -8 & 3 & 1 \\ 3 & 9 & 0 & 0 & 6 & 6 & 2 \\ -1 & -3 & 0 & 1 & 0 & 9 & 3 \end{bmatrix} \quad Echelon\ form$$

$$= \begin{bmatrix} 1 & 3 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1/3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

From Echelon form $x_1 + 3x_2 + 2x_5 = 0$

$x_4 + 2x_5 = 0$

and $x_6 = \frac{1}{3}x_7$

That satisfies $x_1 = -3x_2 - 2x_5$

$x_4 = -2x_5$

And $x_6 = \frac{1}{3}x_7$

Let $x_2 = r,\ x_3 = s,\ x_5 = t,\ x_7 = w$, we get

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{bmatrix} = \begin{bmatrix} -3r-2t \\ r \\ s \\ -2t \\ t \\ \frac{1}{3}w \\ w \end{bmatrix} = r\begin{bmatrix} -3 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + s\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + t\begin{bmatrix} -2 \\ 0 \\ 0 \\ -2 \\ 1 \\ 0 \\ 0 \end{bmatrix} + w\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{3} \\ 1 \end{bmatrix}$$

$$v_1 = \begin{bmatrix} -3 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, v_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, v_3 = \begin{bmatrix} -2 \\ 0 \\ 0 \\ -2 \\ 1 \\ 0 \\ 0 \end{bmatrix}, v_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{3} \\ 1 \end{bmatrix}$$

So the vectors above form the basis for the solution space of A, and is called the null space of A, dimension of the null space is called nullity of A.

Dimension Theorem 2.8. The number of independent rows of a matrix A is called rank of A, that equals the number of non-zero rows with leading entries in the row Echelon form denoted r(A), but nullity represent number of free variables which is numbe of columns without leading entries, Then, n = η(A) + r(A), (Anton and Rorres, 2010).

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Appling dimension theorem n = 5

5= 3 + η(A), so η(A) = 5-3 = 2, such that there are precisely two free variables, x_2 and x_5, so η(A)=2, by another way whwn we know η(A)=2 we can find r(A) by r(A) + η(A) = 5, this lead to r(A) = 5 – η(A) = 5 – 2 = 3 equal the rank of matrix A (Anton and Rorres, 2010).

Example: The sum of rank and nullity of the following matrix is:

rank (A) + nullity (A) = 6, is the numbers of column of A (Anton and Rorres, 2010).

rank (A) = 2 , nullity (A) = 4 .

$$A = \begin{bmatrix} -1 & 2 & 0 & 4 & 5 & -3 \\ 3 & -7 & 2 & 0 & 1 & 4 \\ 2 & -5 & 2 & 4 & 6 & 1 \\ 4 & -9 & 2 & -4 & -4 & 7 \end{bmatrix}$$

$$Echelon\ form\ of\ A = \begin{bmatrix} 1 & 0 & -4 & -28 & -37 & 13 \\ 0 & 1 & -2 & -12 & -16 & 5 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Definition 2.9. A matrix A is said to be in row echelon form if:

1. Rows consisting zeros element entirely must be on the bottom of the matrix.
2. For each nonzero row, the first entry is 1, The first entry is called a leading 1.
3. If a column contains a leading 1, then all other entries in that column are 0.

A matrix A in row echelon form is said to be in reduced row echelon form, or simply reduced, if each corner entry is 1, (Anton and Rorres, 2010).

$$\mathrm{A} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},\ \mathrm{B} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},\ \mathrm{C} = \begin{bmatrix} 1 & * \\ 0 & 1 \end{bmatrix},\ \mathrm{D} = \begin{bmatrix} 1 & * & * \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\mathrm{E} = \begin{bmatrix} 0 & 1 & * & * & * \\ 0 & 0 & 1 & * & * \\ 0 & 0 & 0 & 1 & * \end{bmatrix}, \qquad \mathrm{F} = \begin{bmatrix} 1 & 2 & -1 & 3 \\ 0 & 1 & 2 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

$$Echelon\ form\ \ \mathrm{H} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 1 & -1 & 3 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$R_3 = R_2*(-2)+R_3$

$$reduced\ row\ echelon\ form, rref\ \ \mathrm{H} = \begin{bmatrix} 1 & 0 & 5 & -2 \\ 0 & 1 & -1 & 3 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathrm{K} = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 3 \\ 0 & -1 & -3 \end{bmatrix} \text{ is any matrix}$$

$R_3 = R_2*(1)+R_3$

$$Echelon\ form\ \mathrm{K} = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & 0 \end{bmatrix}$$

$R_1 = R_2*(-2)+R_1$

$$reduced\ row\ echelon\ form, rref\ \mathrm{K} = \begin{bmatrix} 1 & 0 & -5 \\ 0 & 1 & 3 \\ 0 & 0 & 0 \end{bmatrix}$$

2.2. Nullity of The System of Linear Equations.

Assume A is n x m matrix and considers the linear system Ax = b, constructs the augmented matrix B = [A b], then:

- rank (A) = rank(B) = m mean that unique solution x.
- rank (A) = rank(B) $<$ m mean that many solution x.
- rank (A) $<$ rank(B) no solution x.

Now we can use nullity to know the type of the solution of system of linear non-homogeneous equations if a unique solution, no solution and infinite number of solutions (Anton and Rorres, 2010).

Unique solution 2.10.

Consider the system of linear equations.

$x_1 + x_2 + x_3 = 6$

$x_1 - 2x_3 += 4$

$x_2 + x_3 = 2$

$$\mathrm{A} = \begin{bmatrix} 1 & 1 & 1 & 6 \\ 1 & 0 & -2 & 4 \\ 0 & 1 & 1 & 2 \end{bmatrix} \text{ Echenol form for the matrix } \mathrm{A} = \begin{bmatrix} 1 & 0 & 0 & 4 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$x_1 = 4$, $x_2 = 2$, $x_3 = 0$ it mean that there is no free variable therefore the system of linear equation have a unique solution (4,2,0). Now using nullity and the rank of the system (6) we get the same result by Echelon form matrix.

$$\mathrm{D} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & -2 \\ 0 & 1 & 1 \end{bmatrix} \text{ Echelon form for the matrix } \mathrm{D} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

A cording to the dimension theorem we have r(D) = 3 then η(D) = 0 because r(D) + η(D) = 3 order of D, when nullity is zero it mean that there is no free variables, (Anton and Rorres, 2010).

No solution 2.11.

Consider the system of linear equations.

$x_1 + x_2 + x_3 = 6$

$x_1 - 2x_3 = 4$

$2x_1 + x_2 - x_3 = 18$

$$\mathrm{C} = \begin{bmatrix} 1 & 1 & 1 & 6 \\ 1 & 0 & -2 & 4 \\ 2 & 1 & -1 & 18 \end{bmatrix} \text{ Echenol form for the matrix } \mathrm{C} = \begin{bmatrix} 1 & 0 & -2 & 0 \\ 0 & 1 & 3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

We need only to concentrate on the last row of matrix C as it represents the equation

$0x_1 + 0x_2 + 0x_3 = 1$, clearly this equation has no solution. Now using nullity and the rank of the matrix C we get the same result by Echelon form matrix, (Anton and Rorres, 2010).

$$\mathrm{K} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & -2 \\ 2 & 1 & -1 \end{bmatrix} \text{ Echelon form for } \mathrm{K} = \begin{bmatrix} 1 & 0 & -2 \\ 0 & 1 & 3 \\ 0 & 0 & 0 \end{bmatrix}, matrix\ \ KB = \begin{bmatrix} 1 & 1 & 1 & 6 \\ 1 & 0 & -2 & 4 \\ 2 & 1 & -1 & 18 \end{bmatrix}$$

A cording to the dimension theorem we have r(K) = 2, therefore η(K) = 1, because r(K) + η(K) = 3 number of column of k, we have r(B) = 3 and r(K) = 2, when matrix $B = [K, b]$, and r(K)< r(B) the system has no solution ,when nullity is one it mean that there is one free variables that is x_3 , but we can't write x_3 as linear combination for the other variables. (Anton and Rorres, 2010).

Infinite number of solution 2.12.

$+x_2 + x_3 = 6$

$x_1 - 2x_3 = 4$

$2x_1 + x_2 - x_3 = 10$

$$M = \begin{bmatrix} 1 & 1 & 1 & 6 \\ 1 & 0 & -2 & 4 \\ 2 & 1 & -1 & 10 \end{bmatrix} \text{ Echelon form for the matrix } M = \begin{bmatrix} 1 & 0 & -2 & 4 \\ 0 & 1 & 3 & 2 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Not that we have a row of all zeros at the bottom of our matrix, and only we have two pivots x_1 and x_2 are pivots variables, column three has no pivot therefor x_3 is a free variable, the last row of the matrix M represents the equation $0x_1 + 0x_2 + 0x_3 = 0$, that represented by the first two rows of matrix M is, $x_1 - 2x_3 = 4$, $x_2 + 3x_3 = 2$, that $x_1 = 4 + 2x_3$, $x_2 = 2- 3x_3$, when free variable $x_3 = a$, (a is real number), then $x_1 = 4 + 2a$, $x_2 = 2- 3a$, if a = 0, then we get the point (4,2,0), if a = 1, we get the point (6,-1,1) and so on we get infinite solutions (Anton and Rorres, 2010).

Now we use rank of a matrix as a test for linearly independent and invariability. Square matrix $A_{n \times n}$ is invertible (have invers) if and only if its rank equals n.

$$H = \begin{bmatrix} 11 & -21 & 3 \\ 8 & 2 & 1 \\ 16 & -12 & 5 \end{bmatrix} \quad \text{Echelon form of a matrix } H = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

r(H)= 3 = number of column of H, mean that H is invertible, the determinant of H, is exist, and its inverse is exist, means that the column of the matrix are linearly independent, since rank of H, is equals 3, H is not singular and η(H)= 0.

$$D = \begin{bmatrix} 3 & 4 & 5 \\ 6 & 7 & 8 \\ 9 & 10 & 11 \end{bmatrix} \quad \text{Echelon form of a matrix } D = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 2 \\ 0 & 0 & 0 \end{bmatrix}$$

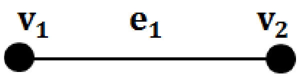
r(D)= 2 not equals the number of column of D, mean that D is not invertible, the determinant of D is not exist, and its inverse is not exist, means that the column of the matrix are not linearly independent, since rank of D is less than 3, D is singular, and η(D) = 1.

2.3. Nullity Application on Some Simple Graphs.

The adjacency matrix of our path graph G_1 with two vertices is.

A= $\begin{matrix} & v_1 & v_2 \\ v_1 & 0 & 1 \\ v_2 & 1 & 0 \end{matrix}$ and its identity matrix is I= $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ we will find xI matrix, xI= $\begin{bmatrix} x & 0 \\ 0 & x \end{bmatrix}$ and, xI –A = $\begin{bmatrix} x & -1 \\ -1 & x \end{bmatrix}$ and determinant of xI-A = $\begin{vmatrix} x & -1 \\ -1 & x \end{vmatrix} = x^2 - 1$ is characteristic polynomial of graph G_1, by solving this equation we get vector $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$,

$x = 1,-1$, therefore, $r(A)=2$, $\eta(A) = 0$.



G_1

Figure 2.2. Path graph $G_1$with two vertices.

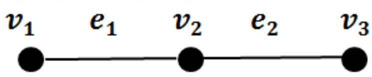
The adjacency matrix of another path graph G_2 is with three vertices,

$$A = \begin{matrix} \\ v_1 \\ v_2 \\ v_3 \end{matrix}\begin{bmatrix} v_1 & v_2 & v_3 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad xI = \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix} \qquad xI - A =$$

$$\begin{bmatrix} x & -1 & 0 \\ -1 & x & -1 \\ 0 & -1 & x \end{bmatrix}$$

$$|xI - A| = \begin{vmatrix} x & -1 & 0 \\ -1 & x & -1 \\ 0 & -1 & x \end{vmatrix} = x^3 - 2x\,,$$ is characteristic polynomial of graph G_2,

$x_1 = 0\,, x_2 = \sqrt{2}\,, x_3 = -\sqrt{2}$, Because one variable equals zero, and two variables are non-zero, therefore, $\eta(A) = 1$ and $r(A) = 2$.



G_2

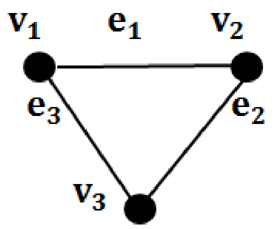
Figure 2.3. Path graph G_2 with three vertices.

If G is a graph and A is adjacency matrix of G rank of G is equals rank of A. $r(G) = r(A)$, and a graph G is said to be singular if its adjacency matrix A is singular, then at least one of the eigenvalue of A is equals zero, the number of zero eigenvalue of matrix A is the nullity of G.

$$A = \begin{matrix} \\ v_1 \\ v_2 \\ v_3 \end{matrix}\begin{bmatrix} v_1 & v_2 & v_3 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}, I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, xI = \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix}, \; xI - A$$

$$= \begin{bmatrix} x & -1 & -1 \\ -1 & x & -1 \\ -1 & -1 & x \end{bmatrix}$$

$$|xI - A| = \begin{vmatrix} x & -1 & -1 \\ -1 & x & -1 \\ -1 & -1 & x \end{vmatrix} = \boldsymbol{x^3 - 3x - 2}$$, is characteristic polynomial of graph G3, by solving this equation we get vectors $\begin{bmatrix} \boldsymbol{x_1} \\ \boldsymbol{x_2} \\ \boldsymbol{x_3} \end{bmatrix} = \begin{bmatrix} \mathbf{2} \\ \mathbf{-1} \\ \mathbf{-1} \end{bmatrix}$, r(A)=r(G) = 3, and η(A) = η(G) = 0



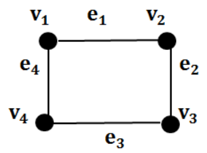
G3

Figure 2.4.Complete graph G3 with three vertices.

$$A = \begin{matrix} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} \begin{bmatrix} v_1 & v_2 & v_3 & v_4 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}, I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad xI = \begin{bmatrix} x & 0 & 0 & 0 \\ 0 & x & 0 & 0 \\ 0 & 0 & x & 0 \\ 0 & 0 & 0 & x \end{bmatrix},$$

$$xI - A = \begin{bmatrix} x & -1 & 0 & -1 \\ -1 & x & -1 & 0 \\ 0 & -1 & x & -1 \\ -1 & 0 & -1 & x \end{bmatrix}, |xI - A| = \begin{bmatrix} x & -1 & 0 & -1 \\ -1 & x & -1 & 0 \\ 0 & -1 & x & -1 \\ 0 & 0 & -1 & x \end{bmatrix} = x^4 -$$

$4x^2 - 4$ Is characteristic polynomial of graph G4**.** By solving this equation we get the vector, $\begin{bmatrix} \boldsymbol{x_1} \\ \boldsymbol{x_2} \\ \boldsymbol{x_3} \\ \boldsymbol{x_4} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{2} \\ \mathbf{-2} \end{bmatrix}$, r(A)=r(G) = 2, and η(A) = η(G) = 2



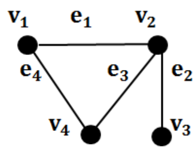
G4

Figure 2.5. Graph G4 with four vertices.

$$A = \begin{matrix} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} \begin{bmatrix} v_1 & v_2 & v_3 & v_4 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix}, I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad xI = \begin{bmatrix} x & 0 & 0 & 0 \\ 0 & x & 0 & 0 \\ 0 & 0 & x & 0 \\ 0 & 0 & 0 & x \end{bmatrix},$$

$$xI - A = \begin{bmatrix} x & -1 & 0 & -1 \\ -1 & x & -1 & 0 \\ 0 & -1 & x & -1 \\ -1 & 0 & -1 & x \end{bmatrix}, |xI - A| = \begin{vmatrix} x & -1 & 0 & -1 \\ -1 & x & -1 & 0 \\ 0 & -1 & x & -1 \\ 0 & 0 & -1 & x \end{vmatrix} = x^4 -$$

$4x^2 - 4x^2 - 2x + 1$ **,** is characteristic polynomial of graph G_5**,** by solving this equation we get the vector $\begin{bmatrix} \boldsymbol{x_1} \\ \boldsymbol{x_2} \\ \boldsymbol{x_3} \\ \boldsymbol{x_4} \end{bmatrix} = \begin{bmatrix} \mathbf{1} \\ \boldsymbol{a} \\ \boldsymbol{b} \\ \boldsymbol{c} \end{bmatrix}$**,** where a, b, c, are real numbers, r(A) = r(G) = 4, and η(A) = η(G) = 0



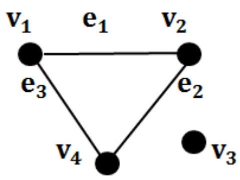
G_5

Figure 2.6. Graph G_5 different structure with four vertices.

$$A = \begin{matrix} X \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} \begin{bmatrix} v_1 & v_2 & v_3 & v_4 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix}, I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad xI = \begin{bmatrix} x & 0 & 0 & 0 \\ 0 & x & 0 & 0 \\ 0 & 0 & x & 0 \\ 0 & 0 & 0 & x \end{bmatrix},$$

$$xI - A = \begin{bmatrix} x & -1 & 0 & -1 \\ -1 & x & 0 & -1 \\ 0 & 0 & x & 0 \\ -1 & -1 & 0 & x \end{bmatrix}, |xI - A| = \begin{vmatrix} x & -1 & 0 & -1 \\ -1 & x & 0 & -1 \\ 0 & 0 & x & 0 \\ -1 & -1 & 0 & x \end{vmatrix} = -x(-x^3 +$$

$3x + 2)$, Is characteristic polynomial of disconnect graph G_6**,** by solving this equation we get vector $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \\ -1 \\ -1 \end{bmatrix}$ because η(A) = 1, and r(A) = 3, therefore n(G) = 1

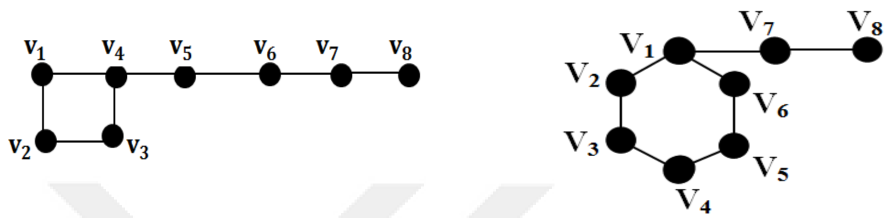


G_6

Figure 2.7. Disconnect graph G_6 with four vertices.

2.4. Relations between Nullity and Graph Structures.

Using nullity we can find a connection between the graph structure and the nullity of graph, in Figure 2.8, the graphs in (G7) and (G8) have the same degree sequence, {3,2,2,2,2,2,2,1},{3,2,2,2,2,2,2,1] respectively, but different nullity, namely in G7 , η(G7) = 2, r(G7) = 6 while in G8 , η(G8) = 0, r(G8) = 8 (Gutman and Bojana, 2009).



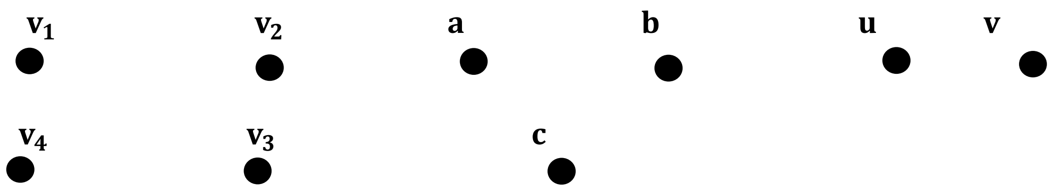
G_7 G_8

Figure 2.8. Relations between nullity and graph structures.

Definition 2.13. A graph G is said to be η-singular or nullity of G is η**,** if the multiplicity of zero (as an eigenvalue) in $S_p(G)$ is η (Sharaf and Rasul 2014).

Lemma 2.14. A graph G with n vertices, η(G) = n, if and only if G is an empty (null) graph (Sharaf and Rasul, 2014).

If A_{4x4} is a matrix of null graph G, then r(A)=0, and η(A)=4, that is order of G, and graph G be 4-singuler.



4-singuler 3-singuler 2-singuler

Figure 2.9. Null graphs.

3. CHEMICAL COMPOUND BOUNDING GRAPHS

In this chapter, we construct several classes of chemical compound graphs, in order to study their nullities and to explain their most important physical property, namely the stability, which is inversely proportional to the nullity (Balakrishnan and Ranganathan, 2012; Gutman, 2008).

The Property such that two isomorphic graphs must either both have the property, or both lack it, is said to be a graph invariant. The question of isomorphism is of a particular interest to chemists. A chemist, who has isolated some compounds from a natural product, will naturally want to know whether they are already known or it is something new. If he determines the various bonding in the molecule, he can draw the structural formula (Gutman, 2008; Balakrishnan and Ranganathan, 2012;).

3.1. Nullity of Chemical Compound Bounding Graphs

The nullity of chemical molecular graphs G is the occurrence of zero as an eigenvalue of its spectrum, denoted by η(G), number of zeros as roots of the polynomial Q(G, x) = |xI − A|, the order of G is equal the sum of its rank and nullity, n= η(G)+r(G), (Ali et all, 2016a).

3.2. Corollary: (End vertex corollary).

If H is subgraph of a graph G, by deleting an end vertex together with the vertex adjacent to it from H, then η(G) = η(H). ■ (Sharaf and Rasul, 2014).

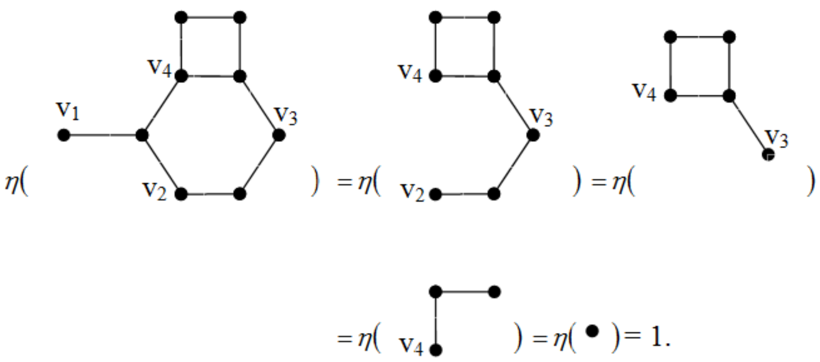


Figure 3.1. Applying End vertex corollary.

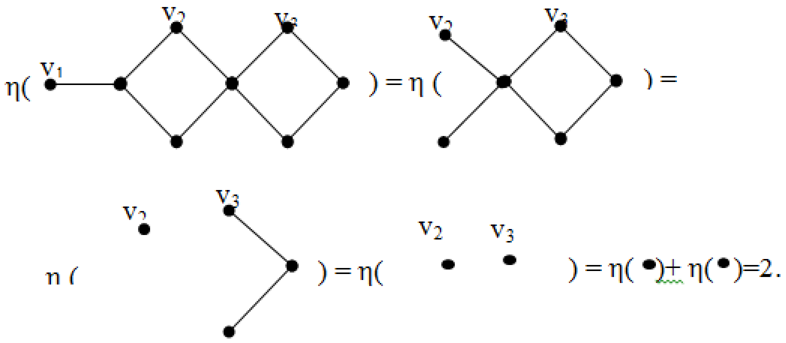


Figure 3.2. Applying End vertex corollary.

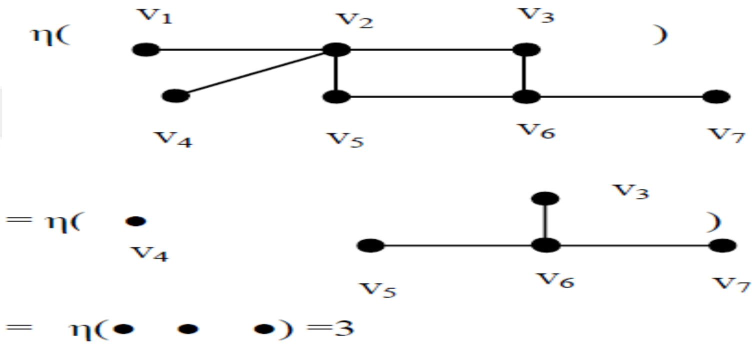
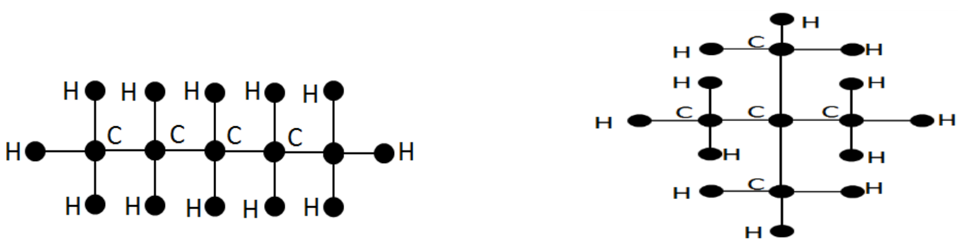


Figure 3.3. Applying corollary 1.

3.3. Isomers Set of Graph.

Two non-isomorphic chemical formula haveing same degree sequence but different structural with different properties are called Isomers, (Balakrishnan and Ranganathan, 2012),

However, the degree of singularity of different isomers my differ such as, in Figure 3.4. (1), η= 7 and Figure 3.4. (2), η= 9.



1 **2**

Figure 3.4. Isomers of C_5H_{12}.

Thus as a chemical property, we mention that the isomer in Figure 3.4. (1) is more stable than that in Figure 3.4. (2).

As a general case, paraffin's have the molecular formula C_nH_{2n+2}. which orders is 3n+2 for n=1, that represent Carbon atom, 2n+2 are Hydrogen atoms. They have size 3n+1 represent bonds between atoms. Hence, for large n, many isomers of the same compound are determined. As a matter of fact, isomers with minimum singularity will appear mostly in nature (Balaban, 1985; Gutman, 2008; Balakrishnan and Ranganathan, 2012).

3.4. Cluster set

A cluster set $\boldsymbol{C}$ in a simple graph G, is bipartite group of vertices of G, each of which has the same set of neighbours. The degree of a cluster set C is the cardinality of its shared set of neighbors, i.e., the common degree of each vertex in the cluster set C. An s-cluster is a cluster set in which each vertex has degree s in it. The order of a cluster set is $|C| = r$, it is often desirable to group elements of a set into disjoint subsets, based on the similarity between the elements in the set (Gutman, 2008; Williams, 2010).

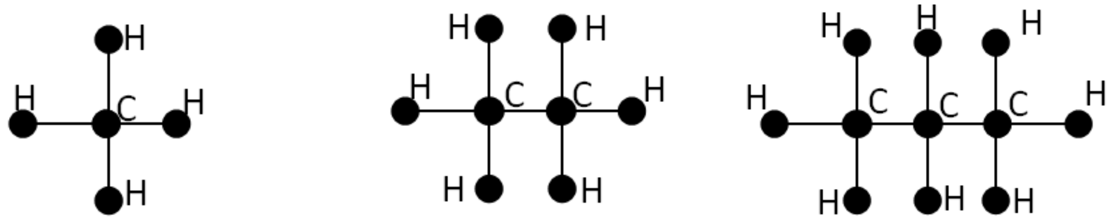
Applying clusters idea as well as end vertex result, we can show that $\eta(C_nH_{2n+2}) \geq n+2$ equality holds for all paraffin compounds whose shape is like Figure 3.4.(1), that is the straight shape is the most stable isomer out of all.

In chemistry of materials, each molecule is constructing from bounding of positive and negative atoms such as Carbon C^{-4}, Oxygen O^{-2}, and Hydrogen $H^{+1}$and so on. Stability is a necessary condition for a structural formulas in organic compounds, because in most cases a molecule formula dose not uniquely represents a single compound see Figure 3.4, say for C_5H_{12} , and different isomers reflect different physical properties, when the groups of atoms that make up the molecules of different isomers are bounded together in fundamentally different ways, they called constitutional (Balakrishnan and Ranganathan, 2012).

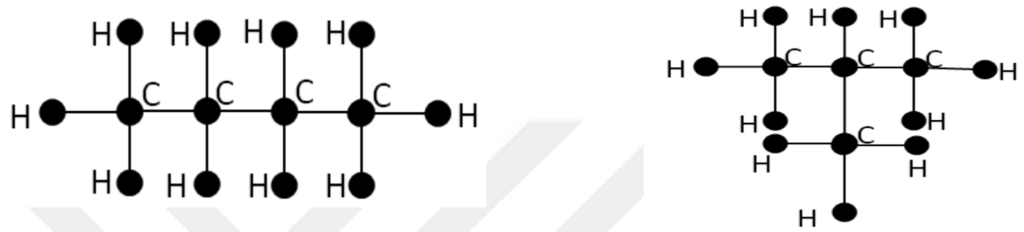
There are two constitutional isomers for C_4H_{10} and three constitutional isomers for C_5H_{10} as indicated in Figures 3.5. And 3.6.

Here, we start with Alkanes C_nH_{2n+2} where each constitutional isomer consist from n atoms of Carbon and 2n+2 atoms of Hydrogen in several graphical shapes with the same degree sequence for the same material. Moreover, we evaluate their nullities without details as indicated in the next figure, where vertices with degree four represent

Carbon atoms and vertices with degree one represent Hydrogen atoms (Balakrishnan and Ranganathan, 2012; Sharaf and Ali, 2014).



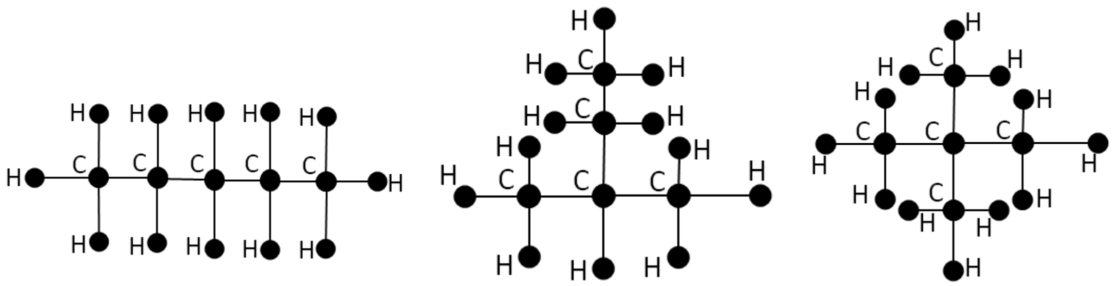
CH_4, $\eta(CH_4) = 3$ C_2H_6, $\eta(C_2H_6) = 4$ C_3H_8, $\eta(C_3H_8) = 5$



Two constitutional isomers of C_4H_{10}, and for both, $\eta(C_4H_{10}) = 6$

Figure 3.5. Chemical graphs for C_nH_{2n+2}, n = 1,2,3 and 4.

It is easy to check that these isomers of C_4H_{10} are non-isomorphic, when n = 5 for C_5H_{12} there exist three non-isomorphic constitutional isomers of pentane, they are depicted in the next figure with their names and nullities. Thus as a chemical property, we mention that the isomers in Figure 3.6 are non-isomorphic (Balakrishnan and Ranganathan, 2012).



n-pentane, $\eta = 7$ 2- methyl butane, $\eta = 7$ 2- dimethyl propane, $\eta = 9$

Figure 3.6. Constitutional isomers of Pentane C_5H_{12}.

The straight chain normal structure is one in which the Carbon atoms induces a path P_n, which is denoted by n – pentane, we prove that, in general nullity of the t , t - timethylpropane is greater than that of n- pentane .

Lemma 3.1. The nullity of the isomer t,t- timethylpropane is greater than the nullity of the n- pentane for constitutional isomers of C_nH_{2n+2} , for $n \geq 5$.

Proof : Appling end vertex corollary n times to the isomers of n- pentane , leaves n+2 isolated vertices while applying it $\lfloor \frac{3n+2}{4} \rfloor$ times to the isomer t,t- timethylpropane , leaves all other remaining vertices to be isolated, then the nullity of t,t- timathylpropane will be $\lfloor 2(3n+2)/4 \rfloor$, which is greater than n+2 , for $n \geq 5$. ■

Corollary 3.2. For any n, $\eta(C_n H_{2n+2}) \geq n+2$.

Proof: The molecular graph $C_n H_{2n+2}$ contain n- pentane isomers for each n with nullity n+2, and all other isomers have nullity not less than that of n- pentane, hence the result holds. ■

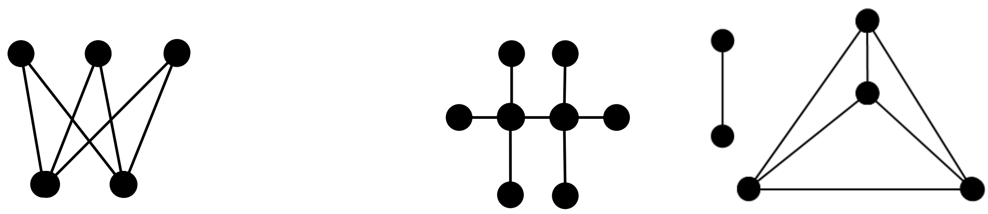
Lemma 3.3. The diameter of the graph of $C_n H_{2n+2}$ is less than or equal to n+1.

Proof: The only isomer with maximum diameter is that of n- pentane with diameter n+1.■

3.5. The Gap between the Nullities of Constitutional Isomers.

In the next we are going to study the nullity of constitutional isomers for some cases of n of the molecule graphs C_nH_{2n+2} for determine the gap between the maximum and minimum nullity of different such constitutional isomers of the graph of C_nH_{2n+2}. First we are interest to introduce some useful definitions.

Definition 3.4. A graph G is called a semi-regular graph if its D(G) degree sequence consist of exactly two elements say r_1 and r_2, (Chartrand and Zhang, 2012).



G_1 , $D(G_1) = \{2,3\}$ G_2 $D(G_2) = \{1,4\}$ G_3 $D(G_3) = \{1,3\}$

Figure 3.7. Semi regular graphs.

Its obvious that a tree T is a semi-regular tree iff deg(u) = deg(v) for each non end vertices u and v of T. Also it is clear that if the diameter of a tree is even then it is center consistes of exactly one vertex.

Definition 3.5. A semi tree T with a central vertex v_0 such that $deg(v_o) = k$, is said to be a symmetric tree if it is symmetric, and also T-v_0 consist of exactly isomorphic subtree.

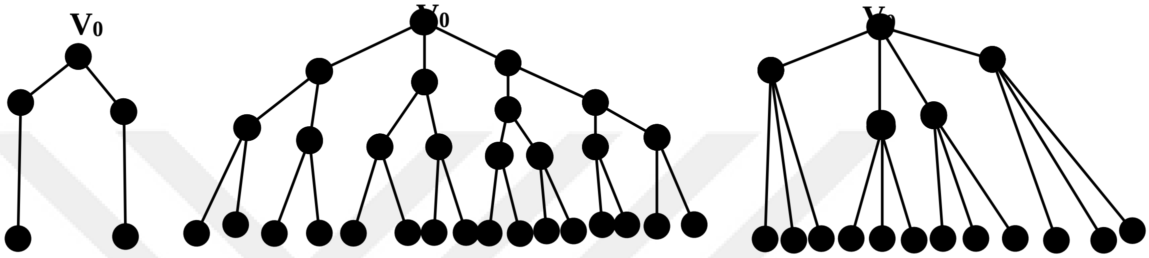
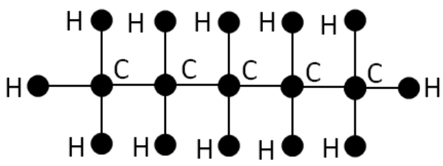


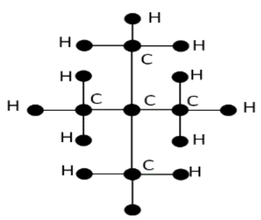
Figure 3.8. Semi symmetric trees.

With benefits of properties of symmetric trees we determine the gap between the nullity of different isomers of molecular graphs. In the following we determine only two constitutional isomers for the molecular graph of $C_{ni}H_{2ni+2}$ one with minimum nullity G_i whose carbon vertices induces a path subgraph P_{ni} namely the n_i pentane and the other T_i where this isomer is a symmetric tree with maximum nullity out of all other constitutional isomers. For i = 0, n_i = 1, is the first number with this property and CH_4 is such a graph with only one isomer say $G_0(C_{no}\ H_{2(no)+2}) \cong T_o(C_{no}\ H_{2(no)+2})$, while for i = 1,2 we have mulecular graphs G_1,T_1 and G_2,T_2 as shown in Figure 3.9. Where vertices of degree 4 represent Carbon atoms, whie of degree 1 are Hydrojeen atoms (Gutman, 2008; Gutman and Bojana, 2009).



G_1

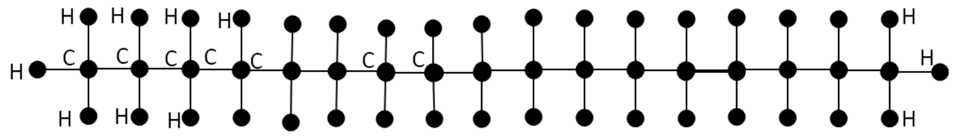
n_1 = 5 ,i = 1 , 5 –pentane,



T_1

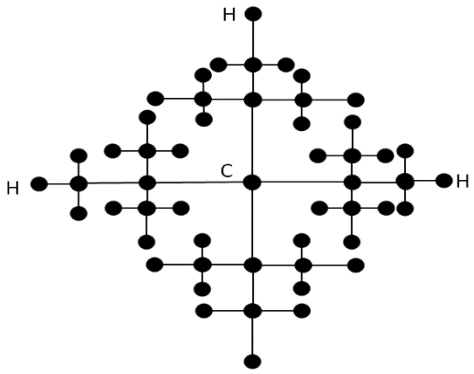
2,2 – dimethyl propane

Figure 3.9. Constitutional isomers G_1,T_1 .of C_5H_{12}.



G_2

The isomer G_2 of $C_{17}H_{36}$ with i = 2, n_2 = 17, 17 – pentane.



T_2

The isomer T_2 of $C_{17}H_{36}$ with 4,4- four methyl propane

Figure 3.10. Constitutional isomers G_2,T_2 of $C_{17}H_{36}$.

It is easy to find the nullity of G_2 which is 19 and of T_2 which is 27.

keeping, the graph T_i to be a symmetric tree, we must identify each end vertex of a symmetric tree T_{i-1} with the central vertex of a star graph $S_{1,3}$ then the order of the tree T_i equals the order of T_{i-1} plus $4(3)^i$, but order of T_0 is 1+4, hence order of T_1 is 1+4+4(3) and order of T_i is, $|Ti|$ = $1+4+4(3)+\ldots.+4(3)^i$

= $1+4[1+3+3^2+\ldots.+3^i]$, which a geometric series with base 3 and its sum is due to the formula $1 + r + r^2 +\ldots + r^i = \frac{r^{i+1}-1}{r-1}$,

$|Ti| = 1 + 4\ (\ \frac{3^{i+1}-1}{2}) = 2(3)^{i+1} -1.$

number of Carbon atoms in T_i is $|C_i|= 1 + 4 +4(3) + \ldots.. + 4(3)^{i-1} = 2(3)^i -1$,

while number of atoms of Hydrogen in T_i is $|H_i| = 4(3^i)$

it is also equals to $2\ |C_i| + 2 = 2(2(3^i) - 1) + 2 = 4(3^i)$.

Lemma 3.6. For any non-negative integer, i, $\eta(G_i) = 2(3)^i + 1$

Proof: $\eta(G_i) = n_i + 2 = \ |C_i| +2 = 2(3^i)-1 + 2 = 2(3)^i +1$. ■

Lemma 3.7. For any positive integer, i, $\eta(G_i) = \eta(G_{i-1}) + 4(3)^{i-1}$

Proof: From Lemma 3.6 we have, $\eta(G_i)= 2(3)^i +1$ and $\eta(G_{i-1})= 2(3)^{i-1} +1$ then, $\eta(G_i) - \eta(G_{i-1}) = 2(3)^i - 2(3)^{i-1} = 2(3)^{i-1}(3-1) = 4(3)^{i-1}$

That is $\eta(G_i) = \eta(G_{i-1})+4(3)^{i-1}$. ■

Lemma 3.8. The nullity of the isomer Ti is defined by $\eta(T_i) = 8(3^{i-1})+ \eta(T_{i-2})$

Proof: Since there exist $4(3^i)$ vertices of Hydrogen hence applying end vertex corollary $\frac{4(3^i)}{3}$ times to obtain (2).(4). (3^{i-1}) isolated vertices, together with a graph isomorphic to T_{i-2} ,

hence $\eta(T_i) = 8(3^{i-1})+\eta(T_{i-2})$. ■

Theorem 3.9. For any non-negative integer, i, $\eta(T_i) = 3^{i+1}$

Proof: We have two cases:

Case 1: Where, i is odd say i = 2k+1,

$\eta(T_i) = 8.3^{i-1}+8.3^{i-3} + \ldots. + 8+1=8 (3^{i-1}+3^{i-3} + \ldots +1) +1$, put i=2k+1

$=8 (9^k+9^{k-1} +\ldots. +1) +1 = 8(\frac{9^{k+1}-1}{8})+1= 9^{k+1} -1+1= 9^{k+1} = 3^{2k+2}= 3^{i+1}$.

Case 2: Where, i is even, put i=2k,

$\eta(T_i) =8 (3^{i-1})+8(3^{i-3})+ \ldots.8(3) +3$

$= 8.3 (3^{i-2}+3^{i-4} +\ldots. +1) +3$

$= 8.3 (3^{2k-2}+3^{2k-4} +\ldots. +1) +3$

$=8.3 (9^{k-1}+9^{k-2} +\ldots. +1) +3$

$= 8.3(\frac{9^k-1}{8}) +3=3.9^k-3+3$

$=3.9^k =3.3^{2k} =3^{i+1}$. ■

Theorem 3.10. The gap between the nullities of the constitutional isomers of $C_{n_i} H_{2n_i+2}$, is 3^i-1,

Proof: The gap between the nullities of the constitutional isomers is.

$|\eta (T_i) - \eta(G_i)| = 3^{i+1} - (2.3^i + 1)=3^i (3-2)-1 = 3^i- 1$. ■

Many results of chapter three are summarized in the next table where,

$|\eta\ (C_i)|$ Is the number of Carbon atoms in $C_{n_i} H_{2n_i+2}$

$|\eta\ (H_i)|$ Is the number of Hydrogen atoms in $C_{n_i} H_{2n_i+2}$

p_i is the order of the graph $C_{n_i} H_{2n_i+2}$

$\eta\ (G_i)$ Is the nullity of the isomer G_i

$\eta\ (T_i)$ Is the nullity of the isomer T_i

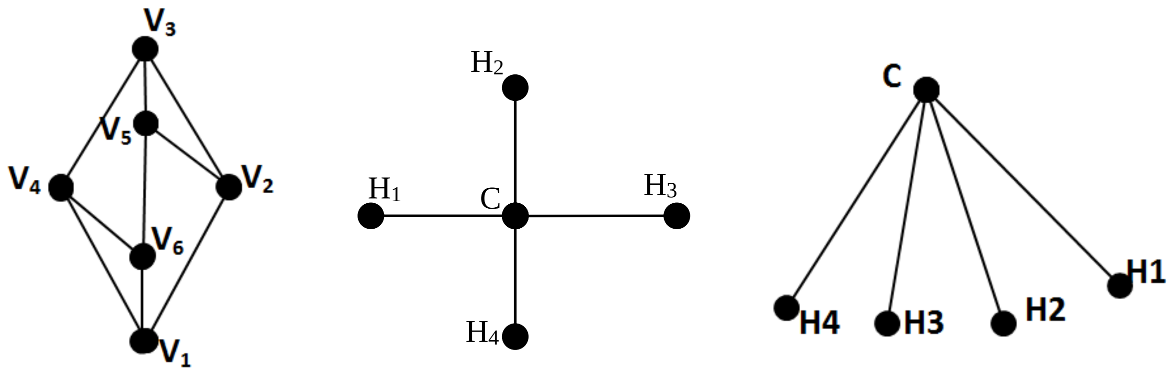
Table 3.1. Some informations of $C_{n_i} H_{2n_i+2}$.

i	n i	(C_i)	(H_i)	Pi	The molecular	$\eta\ (T_i)$	$\eta\ (G_i)$	Gap $\eta\ (T_i) - \eta(G_i)$
0	$n_0 = 1$	1	4	5	CH_4	3	3	0
1	$n_0 = 5$	5	12	17	C_5H_{12}	9	7	2
2	17	17	36	53	$C_{17}H_{36}$	27	19	8
3	53	53	108	161	$C_{53}H_{108}$	81	55	26
4	161	161	324	487	$C_{161}H_{324}$	243	163	80
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.
i=2k	n_{2k}	n_{2k}		$3n_{2k}+2$	$C_{ni}H_{2ni+2}$	3^{i+1}	2.3^i+1	3^i-1
i=2k+1	n_{2k+1}	n_{2k+1}		$3n_{2k+1}+2$	$C_{ni}H_{2ni+2}$	3^{i+1}	2.3^i+1	3^i-1

3.6 The Nullity of Graphs Using Matlab.

Subject to find the degree of singularity(nullity) that η(A(G)), of a graph G by using matlab program we can follow the following way algorithm. the following algorithm of molecule formula of (mithan CH_4) using Matlab program,
(Tutuorials Point, 2014). ***www.tutuorialspoint.com*** .

```
a=[0 1 1 1 1;1 0 0 0 0;1 0 0 0 0;1 0 0 0 0;1 0 0 0 0]

i=eye(5)

b=sym('x')

c=b*i

d=c-a

e=det(d)

f=solve(e)

g=null(a)

h=rank(a)
```



G_1 **$G_2(CH_4)$** **$G_3(CH_4)$**

Figure 3.11. Nullity of graphs using Matlab

$\eta(G_1)=1$	**$\eta(G_2)=3$**	**$\eta(G_3)=3$**
$r(G_1)=5$	**$r(G_2)=2$**	**$r(G_3)= 2$**

```
>> a=[0 1 0 1 0 1;1 0 1 0 0 1;0 0 0 1 1 0;1 1 0 0 1 0;0 0 1 1 0 1;1 1 0 0 1 0]

a =

     0     1     0     1     0     1
     1     0     1     0     0     1
     0     0     0     1     1     0
     1     1     0     0     1     0
     0     0     1     1     0     1
     1     1     0     0     1     0

>> i=eye(6)

i =

     1     0     0     0     0     0
     0     1     0     0     0     0
     0     0     1     0     0     0
     0     0     0     1     0     0
     0     0     0     0     1     0
     0     0     0     0     0     1

>> b=sym('x')

b =

x

>> c=b*i

c =

[ x, 0, 0, 0, 0, 0]
[ 0, x, 0, 0, 0, 0]
[ 0, 0, x, 0, 0, 0]
[ 0, 0, 0, x, 0, 0]
[ 0, 0, 0, 0, x, 0]
[ 0, 0, 0, 0, 0, x]

>> d=c-a

d =

[  x, -1,  0, -1,  0, -1]
[ -1,  x, -1,  0,  0, -1]
[  0,  0,  x, -1, -1,  0]
[ -1, -1,  0,  x, -1,  0]
[  0,  0, -1, -1,  x, -1]
[ -1, -1,  0,  0, -1,  x]

>> e=det(d)

e =

x^6 - 7*x^4 - 5*x^3 + 3*x^2 + 2*x

>> f=solve(e)
f =

         0
        -1
        -2
                                   1/((3^(1/2)*i)/2 + 1/2)^(1/3) + ((3^(1/2)*i)/2 + 1/2)^(1/3) + 1
 (3^(1/2)*(1/((3^(1/2)*i)/2 + 1/2)^(1/3) - ((3^(1/2)*i)/2 + 1/2)^(1/3))*i)/2 - 1/(2*(3^(1/2)*(i/2) + 1/2)^(1/3)) - ((3^(1/2)*i)/2
 1 - 1/(2*(3^(1/2)*(i/2) + 1/2)^(1/3)) - ((3^(1/2)*i)/2 + 1/2)^(1/3)/2 - (3^(1/2)*(1/((3^(1/2)*i)/2 + 1/2)^(1/3) - ((3^(1/2)*i)/2

>> h=rank(a)

h =

         5
```

```
a=[0 1 0 1 0 1;1 0 1 0 0 1;0 0 0 1 1 0;1 1 0 0 1 0;0 0 1 1 0 1;1 1 0 0 1 0]
i=eye(6)
b=sym('x')
c=b*i
d=c-a
e=det(d)
f=solve(e)
h=rank(a)
```

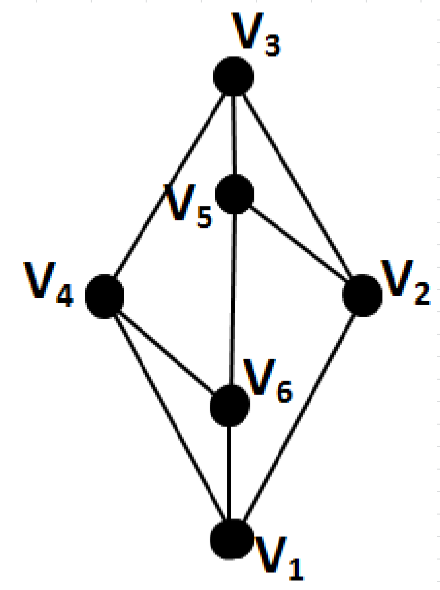


Figure 3.12. Matlab program output

```
>> a=[0 1 1 1 1;1 0 0 0 0;1 0 0 0 0;1 0 0 0 0;1 0 0 0 0]

a =

     0     1     1     1     1
     1     0     0     0     0
     1     0     0     0     0
     1     0     0     0     0
     1     0     0     0     0

>> i=eye(5)

i =

     1     0     0     0     0
     0     1     0     0     0
     0     0     1     0     0
     0     0     0     1     0
     0     0     0     0     1

>> b=sym('x')

b = x
>> c=b*i
c =

[ x, 0, 0, 0, 0]
[ 0, x, 0, 0, 0]
[ 0, 0, x, 0, 0]
[ 0, 0, 0, x, 0]
[ 0, 0, 0, 0, x]

>> d=c-a

d =

[  x, -1, -1, -1, -1]
[ -1,  x,  0,  0,  0]
[ -1,  0,  x,  0,  0]
[ -1,  0,  0,  x,  0]
[ -1,  0,  0,  0,  x]

>> e=det(d)

e =

x^5 - 4*x^3

>> f=solve(e)

f =

   0
   0
   0
   2
  -2


>> g=null(a)

g =

        0         0         0
  -0.5000   -0.1081   -0.6988
   0.5000    0.6988   -0.1081
  -0.5000    0.1081    0.6988
   0.5000   -0.6988    0.1081

>> h=rank(a)

h = 2
```

```
a=[0 1 1 1 1;1 0 0 0 0;1 0 0 0 0q
i=eye(5)
b=sym('x')
c=b*i
d=c-a
e=det(d)
f=solve(e)
g=null(a)
h=rank(a)
```

Tre

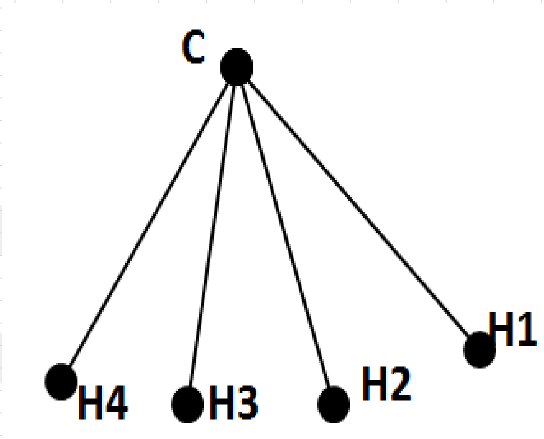
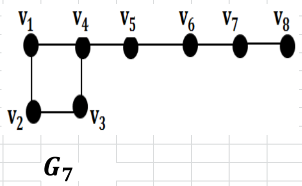


Figure 3.13. Matlab Program output.

```
>> a=[0 1 0 1 0 0 0 0;1 0 1 0 0 0 0 0;0 1 0 1 0 0 0 0;1 0 1 0 0 0 0 0;0 0 0 1 0 1 0 0;0 0 0 0 1 0 1 0;0 0 0 0 0 1 0 1;0 0 0 0 0 0 1 0]

a =

   0   1   0   1   0   0   0   0
   1   0   1   0   0   0   0   0
   0   1   0   1   0   0   0   0
   1   0   1   0   0   0   0   0
   0   0   0   1   0   1   0   0
   0   0   0   0   1   0   1   0
   0   0   0   0   0   1   0   1
   0   0   0   0   0   0   1   0
```

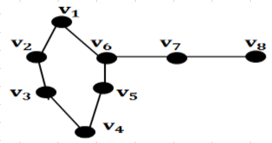



```
>> i=eye(8)

i =

   1   0   0   0   0   0   0   0
   0   1   0   0   0   0   0   0
   0   0   1   0   0   0   0   0
   0   0   0   1   0   0   0   0
   0   0   0   0   1   0   0   0
   0   0   0   0   0   1   0   0
   0   0   0   0   0   0   1   0
   0   0   0   0   0   0   0   1

>> b=sym('x')

b =

x

>> c=b*i

c =

[ x, 0, 0, 0, 0, 0, 0, 0]
[ 0, x, 0, 0, 0, 0, 0, 0]
[ 0, 0, x, 0, 0, 0, 0, 0]
[ 0, 0, 0, x, 0, 0, 0, 0]
[ 0, 0, 0, 0, x, 0, 0, 0]
[ 0, 0, 0, 0, 0, x, 0, 0]
[ 0, 0, 0, 0, 0, 0, x, 0]
[ 0, 0, 0, 0, 0, 0, 0, x]

>> d=c-a

d =

[  x, -1,  0, -1,  0,  0,  0,  0]
[ -1,  x, -1,  0,  0,  0,  0,  0]
[  0, -1,  x, -1,  0,  0,  0,  0]
[ -1,  0, -1,  x,  0,  0,  0,  0]
[  0,  0,  0, -1,  x, -1,  0,  0]
[  0,  0,  0,  0, -1,  x, -1,  0]
[  0,  0,  0,  0,  0, -1,  x, -1]
[  0,  0,  0,  0,  0,  0, -1,  x]

>> e=det(d)

e =

x^8 - 7*x^6 + 13*x^4 - 4*x^2

>> f=solve(e)

f =

    2
    0
    0
   -2
  5^(1/2)/2 + 1/2
  5^(1/2)/2 - 1/2
  1/2 - 5^(1/2)/2
 - 5^(1/2)/2 - 1/2

>> rref(a)

ans =

   1   0   1   0   0   0   0   0
   0   1   0   0   0   0   0   1
   0   0   0   1   0   0   0  -1
   0   0   0   0   1   0   0   0
   0   0   0   0   0   1   0   1
   0   0   0   0   0   0   1   0
   0   0   0   0   0   0   0   0
   0   0   0   0   0   0   0   0
```

```
>> det(a)

ans =

     0
```

```
>> rank(a)

ans =

     6
```

Figure 3.14. Matlab program output



G_8

```
>> a=[0 1 0 0 0 1 0 0;1 0 1 0 0 0 0 0;0 1 0 1 0 0 0 0;0 0 1 0 1 0 0 0;0 0 0 1 0 1 0 0;1 0 0 0 1 0 1 0;0 0 0 0 0 0 0 1;0 0 0 0 0 0 1

a =

   0   1   0   0   0   1   0   0
   1   0   1   0   0   0   0   0
   0   1   0   1   0   0   0   0
   0   0   1   0   1   0   0   0
   0   0   0   1   0   1   0   0
   1   0   0   0   1   0   1   0
   0   0   0   0   0   0   0   1
   0   0   0   0   0   0   1   0

>> i=eye(8)

i =

   1   0   0   0   0   0   0   0
   0   1   0   0   0   0   0   0
   0   0   1   0   0   0   0   0
   0   0   0   1   0   0   0   0
   0   0   0   0   1   0   0   0
   0   0   0   0   0   1   0   0
   0   0   0   0   0   0   1   0
   0   0   0   0   0   0   0   1

>> b=sym('x')

b =

x

>> c=b*i

c =

[ x, 0, 0, 0, 0, 0, 0, 0]
[ 0, x, 0, 0, 0, 0, 0, 0]
[ 0, 0, x, 0, 0, 0, 0, 0]
[ 0, 0, 0, x, 0, 0, 0, 0]
[ 0, 0, 0, 0, x, 0, 0, 0]
[ 0, 0, 0, 0, 0, x, 0, 0]
[ 0, 0, 0, 0, 0, 0, x, 0]
[ 0, 0, 0, 0, 0, 0, 0, x]

>> d=c-a

d =

[  x, -1,  0,  0,  0, -1,  0,  0]
[ -1,  x, -1,  0,  0,  0,  0,  0]
[  0, -1,  x, -1,  0,  0,  0,  0]
[  0,  0, -1,  x, -1,  0,  0,  0]
[  0,  0,  0, -1,  x, -1,  0,  0]
[ -1,  0,  0,  0, -1,  x, -1,  0]
[  0,  0,  0,  0,  0,  0,  x, -1]
[  0,  0,  0,  0,  0,  0, -1,  x]

>> e=det(d)

e =

x^8 - 7*x^6 + 15*x^4 - 13*x^2 + 4

>> f=solve(e)

f =

    2
    1
    1
    1
   -1
   -1
   -1
   -2
```

```
>> det(a)

ans =

   4
```

```
>> rank(a)

ans =

   8
```

```
>> rref(a)

ans =

   1   0   0   0   0   0   0   0
   0   1   0   0   0   0   0   0
   0   0   1   0   0   0   0   0
   0   0   0   1   0   0   0   0
   0   0   0   0   1   0   0   0
   0   0   0   0   0   1   0   0
   0   0   0   0   0   0   1   0
   0   0   0   0   0   0   0   1
```

Figure 3.15. Matlab program output

4. CONCLUSION

Graph theory has become an important discipline in its own right because of its applications to Computer Science, Communication Networks, and Combinatorial optimization through the design of efficient algorithms. It has seen increasing interactions with other areas of mathematics.

We know there are many interactions between the theories of graph spectra and other branches of mathematics, especially to linear algebra. Many results and techniques from the theory of graph spectra can be applied for the foundations and development of matrix theory. Relations between eigenvalues of graphs and combinatorial optimization have been known for last twenty years. There are several objects which are nowadays naturally described as graphs.

Firstly a graph is an ordered pair of vertices connected together by edges, we consider finite connected undirected simple graphs with labeled vertices.

After that we studied how we can find the characteristic polynomial of G by A(G) that represent G, because A(G) is symmetric matrix its eigenvalue λ_1, λ_2, ..., λ_p are a real numbers.

During our work we defined when A(G) of graph G is singular, it means that determenat of A(G) equals to zero,therefore graph G is singular .

According to our work, we focused on the nullity of graphs, that occurrence of zeros in the spectrum of G.

We study some applications on graph spectra such as the relation between the degree of singularity and the instability of the molecular formula of chemical compounds graphs.

Finally, the thesis includes some tables on the nullity of some chemical graphs, and formulas to determine the nullity of some isomer chemical graphs.

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APPENDIX
EXTENDED TURKISH SUMMARY
GENİŞLETİLMİŞ TÜRKÇE ÖZET

Uygulamalı Matematiğin bir dalı olan graf(çizge) teorisi mühendislikten fen bilimlerine, işletmeden sosyal bilimlere kadar bir çok uygulamaya sahiptir. Uygulamada karşılaşılan birçok problem graflar vasıtasıyla modellenerek çözümleri bulunmaya çalışılır. Çizge teorisi (graph theory) literatürde çok farklı disiplinlerin çalışma alanına girmektedir. Sosyolojiden matematiğe, işletmeden bilgisayar bilimlerine kadar farklı alanlarda kullanılmaktadır. Örneğin bilgisayar bilimlerinin altında ayrık matematik (discrete math) veya endüstri mühendisliği altında yön eylem çalışmaları (operations research) veya matematiğin bir çalışma alanı olarak karşılaşılabilir. Çizge teorisi temel olarak bir problemin kenar (edge) ve düğümler (node) ile modellenmesi ve bu modelin bir çizge şeklinde gösterilmesi ilkesine dayanmaktadır. Çizge teorisinde tanımlı olan bazı özellikler bu modelin çözümüne ve dolayısıyla gerçek problemin çözümüne yardımcı olmaktadırlar. Yani çizge teorisinin işe yaraması için öncelikle gerçek dünyadan bir problem çizge olarak modellenir, bu model çözülür ve daha sonra gerçek dünyaya uygulanır.

Graf(Çizge) teorisi, 1700′ lü yılların meşhur problemi olan “Königsberg’in 7 köprüsü” probleminin çözümüyle doğmuştur. Königsberg şehri Pregel nehrinin kıyısına kurulmuş ve yedi ayrı köprü ile birbirine bağlanmış dört farklı bölümden oluşmaktadır. Zamanla insanlar kendilerine, aynı köprüden bir kez daha geçmemek üzere tüm şehri dolaşmanın mümkün olup olmadığı sorusunu sormuşlardır. Ancak hiç kimse böyle bir rota çizemedi, dönemin meşhur matematikçilerinden biri olan Leonhard Euler’ de dahil, fakat Euler bunun neden mümkün olamayacağını ispatlayabilmiştir. Euler, problemin ispatı için şekli daha basit bir hale getirmiştir, bunun için köprüleri çizgiler ve şehir parçalarınıda noktalar halinde ifade etmiştir, bunun sonucu olarak aşağıdaki şekil ortaya çıkmıştır. Euler böyle bir gezinin mümkün olabilmesi için her noktada buluşan çizgilerin toplam sayısının çift rakam olması gerektiği kanısına varmıştır, bu sayede bir noktaya ulaşmak için köprülerden birisi, çıkmak içinse diğeri kullanılacaktı, ancak ortada bir istisna vardı, başlangıç ve bitiş noktaları. Başlangıç ve bitiş noktalarının farklı olduğu durumlarda bu iki noktanın sadece tek bir çizgi ile diğer noktalara bağlı olması gerekiyordu, başlangıç ve bitiş noktalarının aynı olduğu durumlarda ise her noktanın çift sayıda köprüye ihtiyacı vardır. Bütün bu düşünceler ışığında Euler genel bir teoremi ortaya çıkartmıştır, bu teoreme göre böyle bir gezintiyi mümkün kılabilmek için sistemdeki her bir noktaya ulaşan toplam çizgi saysının çiftolması yada en fazla iki noktaya ulaşan toplam çizgi sayısının tek olması zorunluydu. 1736`da Euler`in incelemeleri böyle bir gezintinin mümkün olmadığını kanıtlamış ve bu tür dolaşmayı mümkün kılacak çizgelerin şu özelliklere sahip olmaları gerektiğini göstermiştir, birleşik bir çizgenin bütün elemanlarını bir ve yalnız bir kez kullanarak dolaşmak için o çizgenin tek dereceli düğümlerinin sayısı, eğer varsa, iki olmalıdır, tek dereceli düğümler dolaşmanın başlangıç ve bitiş düğümleridir, çizgede böyle düğümler yoksa dolaşmaya herhangi bir düğümden başlanabilir. Çözümün temelinde yatan düşünce şudur, bir düğüm, başlangıç ya da bitiş düğümü değilse o düğüme gelen kişinin turu tamamlayabilmek için oradan ayrılması gerekecektir. Dolayısıyla bu tip düğümler çift dereceleri olmalıdır, oysa tek dereceli bir düğüme ikinci kez gelen bir kişi çıkış yolu bulamayacaktır. Dolayısıyla bu düğüm ya gezintinin bitiş düğümü olmalıdır ya da başlangıç düğümü olarak seçilmelidir ki ikinci gelişte çıkış yolu bulunabilsin, buna göre tek dereceli düğüm sayısı ikiden fazlaysa gezinti tamamlanamayacaktır. Yürüyüşün sonunda başlangıç noktasına dönülebilmesi içinse bütün düğümler çift dereceli olmalıdır, böylece, başlangıç ve bitiş düğümü aynı olan ve her bir elemanı sedece ve en az bir kez içeren turlara "Euler turu" ve Euler turu içeren çizgelere de "Euler çizgesi" denmiştir.

Yine 19. Yüzyılın en meşhur problemlerinden biri olan "Oniki yüzlü bir şeklin köşelerinin her birine bir kere uğramak koşulu ile tüm alanda devir yapmak mümkün müdür?" problem de İrlandalı bir fizikçi, matematikçi ve astronom Sir William Rowan Hamilton tarafından graf teorisi yardımıyla çözülebilmiştir. Bu iki çalışmadan sonra, Graf Teorisi 20. Yüzyılın ilk yıllarından itibaren uygulamalı matematiğin yeni bir dalı olarak ortaya çıkmıştır.

Graf teorinin diger matematik bilim dallarıyla ilişkisi de son yıllarda bir çok araştırmacının dikkatini çekmiştir. Graf teorinin lineer cebirle ilişkisi son kırk yıldır literatürde çalışılmaya başlanmış ve "Lineer Cebirsel Graf Teori" nin doğuşu gerçekleşmiştir. İşte bu çalışmada Lineer Cebirsel Graf Teorinin bir konusu olan grafların sıfırlıkları ve bu sıfırlıkların kimyasal graf teoride kimyasal özelliklerle ilişkisiyle ilgili son zamanlarda literatürde yapılan çalışmaların özet bir sunumundan ibarettir.

Çalışmanın ilk bölümünde temel tanım ve teoremler verilerek graflar ve matrisler arasındaki ilişki ortaya konulmuştur. Ayrıca konuyla ilgili bir literature taraması verilmiştir.

İkinci bölümü sıfırlık kavramının lineer cebir bakımından incelenmesi ve bu sıfırlık kavramının graf teorisine nasıl taşındığıyla ilgili olup, konunu daha iyi pekişmesi için seçilen bazı özel graf sınıfları için sıfırlıkların bazı graf değişmezleri ile ilgili ilişkisiyle ilgili bazı sonuçlar yine bu ikinci bölümde ifade edilmiştir.

Üçüncü bölüm kimyasal grafların sıfırlıkları ve bu sıfırlıkların bukimyasal grafların kimyasal özellikleri arasındaki ilişki üzerinedir. Özellikle son tepe lemmasının nasıl uygulandığıyla ilgili örnekler gerçekten çok ilgi çekicidir. İzomer grafların sıfırlıklarının ayrı olabileceği gerçekten kimyasal açıdan önem arzeder. Yine yapısal izomerler ve sıfırlıklar arasındaki ilşkiyle ilgili daha ileri çalışmaların sonuçları bu bölümde ifade edimiştir. Ayrıca sıfırlıkların Matlab programı yardımıyla nasıl hesaplanacağıyla ilgili bazı örnekler yine bu bölümde sunulmuştur.

Sonuç olarak grafların matrislerle değişik temsillerinden ve bu temsillerin lineer cebirsel özelliklerinin incelenmesi ve konunun daha açık ve anlaşılır sonuçlarla ifade edilmesi için daha bir çok çalışmaya ihtiyaç duyulduğu aşikardır.

CURRICULUM VITAE

He was born in Zakho, Duhok from Iraq, in 1964. He went to University of Mosul in 1984 until 1988 of College of Science and got Bachelor's Degree, in Mathematics Department. In addition, about ten years he was research assistant at University of Polytechnic of Duhok. At February 2014, he started his master study in Van Yüzüncü Yıl University, Van-Turkey.

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