Some Problems in Graph Theory

STUDIES ON THE SPECTRUM AND THE ENERGY OF GRAPHS

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By

INDULAL G.

Department of Mathematics

Cochin University of Science and Technology

Cochin - 682 022

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Certificate

This is to certify that the thesis entitled '**Studies on the Spectrum and the Energy of Graphs**' submitted to the Cochin University of Science and Technology by Sri. Indulal G. for the award of the degree of Doctor of Philosophy under the Faculty of Science is a bonafide record of studies carried out by him under my supervision in the Department of Mathematics, Cochin University of Science and Technology. This report has not been submitted previously for considering the award of any degree, fellowship or similar titles elsewhere.

Dr. A.Vijayakumar

(Supervisor)

Reader, Department of Mathematics

Cochin University of Science and Technology

Cochin-682 022, Kerala.

Cochin

29/03/2007

Declaration

I, Indulal G. hereby declare that this thesis entitled **'Studies on the Spectrum and the Energy of Graphs'** contains no material which had been accepted for any other Degree, Diploma or similar titles in any University or Institution and that to the best of my knowledge and belief, it contains no material previously published by any person except where due references are made in the text of the thesis.

Indulal G.
Research Scholar
(Registration No. 2261)
Department of Mathematics
Cochin University of Science and Technology
Cochin-682 022, Kerala.

Cochin
29/03/2007

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Indulal G.

STUDIES ON THE SPECTRUM AND THE ENERGY OF GRAPHS

Contents

Chapter 1

Introduction

The origin of 'Graph Theory' dates back to more than two hundred and seventy years when the famous Swiss Mathematician Leonhard Euler (1707 - 1783) solved the 'Konig̈sberg Bridge Problem' in a talk entitled 'The solution of a problem relating to the geometry of position' presented at the St.Petersberg Academy on 26^{th} August, 1735. Since then, the subject has grown both in its theory and its varied applications, initiated by the works of such greats as W.R. Hamilton, De Morgan, A. Cayley and P. J. Heawood. The celebrated '4 Color Problem' which was a major unsolved problem since 1852 and its unique method of solution using computers in 1976 - the first of its kind in Mathematics, also belongs to Graph Theory. In 1874, A. Cayley realized that the problem of finding the number of different paraffines with the formula C_nH_{2n+2} is essentially the same as the problem of counting the number of unrooted trees with n vertices, where no vertex has valency exceeding four. But it was J. J. Sylvester who first used the term 'graph' in his celebrated paper 'Chemistry and Algebra' in 1877.

The first book on graph theory was written by D. König [61]. Later, C. Berge [13], O. Ore [74] and F. Harary [48] also wrote the first set of books in this subject. N.L. Biggs, E. K. Lloyd and R. J. Wilson [15] has discussed in detail, with the extracts of original work, the growth of graph theory. F. S. Roberts [80] has dealt with a variety of applications of graphs in engineering, technology, biological sciences, archeology, ecology, planning etc. This includes its applications in transportation problems, communication, study of food webs in ecology, round - robin tournament in tennis, the theory of structural balance in sociology etc. In [12], connections of graph theory with other branches of mathematics such as number theory, coding theory are discussed.

The growth of Computer Science and the resulting information revolution has tremendous impact in the application of graphs (networks) also [2]. One such significant theme is the study of the 'diameter of the world wide web'[1]. This can be termed as the twenty first century application of graph theory. The world wide web is a network of web pages containing information linked together by hyperlinks from one page to another [52]. The study of this, opened up a new concept called - the small world phenomenon, which lead J. M. Kleinberg [60] to win the prestigious Nevanlinna prize in 2006. Researchers have in recent years developed a variety of techniques and models to help us understand or predict the behavior of the networked systems such as internet, social networks and biological networks [72].

Volumes have been written on the rich theory and the very many application of graphs. This thesis entitled **'Studies on the Spectrum and the Energy of Graphs'** is a humble attempt at making a small addition to the vast ocean of results in graph theory. We shall list below only some very significant developments in the theory of eigenvalues and energy of graphs.

A non-pictorial representation of a graph is effected by its adjacency matrix. So during the 1950s the question arose as to how the well developed theories of matrices and graphs could be combined to evolve a new approach in applying matrix techniques to graphs. The first concept which came to the minds of many researchers in graph theory was the eigenvalues of a matrix. The eigenvalues of a graph are precisely the eigenvalues of its adjacency matrix. Most of the early results in this were concerned with the relation between spectral and structural properties of graphs.

The first significant result on the concept of the characteristic polynomial was due to Sachs [82] and is usually known as 'Sach's theorem'. The specialization of a deep theorem on non negative matrices proved by Perron and Frobenius resulted in the 'Perron-Frobenius theorem' [34] on the eigenvalues of a connected graph. The 'Pairing theorem' of Coulson and Rushbrooke [20] on the eigenvalues of a bipartite graph has some implications in chemistry also. For a detailed account of various other results on the eigenvalues of graphs we refer to [27] and [88]. Recent developments in graph spectra are also available in the spectral graph theory home page, www.sgt.pep.ufrj.br

A resurgence was seen in the study of the 'chemical applications of graph theory' which was initiated by E. Hückel in his molecular orbital theory during 1930s. In quantum chemistry the skeleton of certain non-saturated hydrocarbons are represented by graphs. The energy levels of electrons in such a molecule are, in fact, the eigenvalues of the corresponding graph. The stability of the molecules as well as other chemically relevant facts are closely connected with the graph spectrum and the corresponding eigenvectors. For more information on chemical application of graph theory see [5, 96].

The molecular orbital energy levels $\mathcal{E}_j$ of the $\pi-$ electrons in conjugated molecules are related to the eigenvalues of the corresponding molecular graph by a linear function

$$\mathcal{E}_j = \alpha + \beta\lambda_j$$

within the Hückel Molecular Orbital (HMO) theory where $\lambda_j' s$ are the eigenvalues of the corresponding graph[19, 37] and $\alpha,\ \beta$ are the standard HMO parameters [43]. Thus, the total $\pi-$ electron energy, $\mathcal{E}_\pi$ is uniquely determined by the topology of the corresponding molecule via the eigenvalues of its molecular graph and it is computed as

$$\begin{aligned}\mathcal{E}_\pi &= \alpha n_e + \beta \sum_{i=1}^{p} g_i\lambda_i \\ &= \alpha n_e + \beta\mathcal{E}.\end{aligned}$$

where n_e is the number of $\pi-$ electrons, g_i is the occupation number of the i^{th} molecular orbital and $\lambda_i,\quad i = 1, 2, ..., p$ are the eigenvalues of the corresponding molecular graph. The nontrivial part of the above expression is $\mathcal{E}$. For the vast majority of conjugated molecules, $\mathcal{E}$ can be transformed into

$$\mathcal{E} = \sum_{i=1}^{p} |\lambda_i| \, .$$

Motivated by this connection between total $\pi-$ electron energy and eigenvalues of the corresponding graph, I.Gutman [39] in 1978 introduced the concept of 'graph energy' as the sum of the absolute values of the eigenvalues of G. The introduction of this concept resulted in the discovery of numerous novel results, some of which have chemical relevance too.

Other aspects of the interplay between Algebra and Graph Theory involving the eigenvalues has been dealt with in detail by C.D. Godsil [35] and N.L. Biggs [14]. O.E. Polansky [43] has also discussed in detail several other chemical applications of graph theory such as Hosoya index, thermodynamic stability of conjugated molecules and matching polynomials.

This thesis is mainly concerned with the eigenvalues of graphs and graph energy.

1.1 Basic definitions and lemmas

We use the following terminology, definitions and lemmas from [3, 24, 36, 48, 83, 84, 97].

Definition 1. *A graph G is a pair (V, E) where $V = V(G)$ is a nonempty set of objects with $V(G) = \{v_1, v_2, \ldots, v_p\}$ called* ***vertices*** *and $E = E(G)$, a set of unordered pairs of distinct vertices of G called* ***edges****. $|V|$ is called its* ***order*** *denoted by p and $|E|$, the* ***size****, denoted by q. A graph G of order p and size q is referred to as a (p, q) graph. A graph $H = (V', E')$ is said to be a* ***subgraph*** *of G if $V' \subseteq V$ and $E' \subseteq E'$. It is said to be a* ***spanning subgraph*** *if $V' = V$. A subgraph H of G is said to be an* ***induced subgraph*** *of G if each edge of G having its end vertices in $V(H)$ is also an edge of H. The 'n' disjoint copies of a graph G is denoted by nG.*

Definition 2. *Let $G = (V, E)$ be a (p, q) graph. If $\{u, v\} \in E(G)$, then u and v are said to be the end vertices of the edge $e = \{u, v\}$. Two vertices $u, v \in V(G)$ are said to be* ***adjacent*** *if $\{u, v\} \in E(G)$. A vertex u is said to be* ***incident*** *with an edge e if u is an end vertex of e. Two edges e and e' are said to be adjacent if they have a common end vertex. The number of vertices adjacent to v is called its*

degree *denoted by* $deg(v)$. *A vertex* v *of* G *with* $deg(v) = 1$ *is a* ***pendant vertex***. *The set of vertices adjacent to* v *is called the* ***open neighborhood*** *of* v *denoted by* $N(v)$. *The set* $N(v) \bigcup \{v\}$ *is called the* ***closed neighborhood*** *of* v *denoted by* $N[v]$.

Definition 3. *A graph* G *is said to be* $r-$***regular*** *if all the vertices of* G *have the same degree* r. *A* $3-$ *regular graph is called a* ***cubic graph***.

Definition 4. *Two graphs* $G = (V, E)$ *and* $H = (V', E')$ *are said to be* ***isomorphic*** *if there exists a bijection from* V *to* V' *preserving adjacency and is written as* $G = H$.

Definition 5. *Let* G *be a graph. A* ***path*** *in* G *is an alternating sequence of distinct vertices and edges, beginning and ending in vertices such that each edge is incident with the vertices preceding and following it. A path starting at* u *and ending at* v *is a* $u - v$ *path. A graph* G *is* ***connected*** *if there exists a* $u - v$ *path for every* $u,\ v \in V(G)$. *A graph which is not connected is a* ***disconnected graph***. *A maximal connected subgraph of* G *is called a* ***component*** *of* G. *A path starting and ending in the same vertex is a* ***cycle***. P_n *and* C_n *respectively denote the path and the cycle on* n *vertices.*

Definition 6. *A graph* G *is complete if every pair of distinct vertices of* G *are adjacent in* G. *A* ***complete graph*** *of order* p *is denoted by* K_p. *A graph* G *is a* ***bipartite graph*** *if* $V(G)$ *can be partitioned into two nonempty sets* U *and* U' *such that each edge of* G *has one end vertex in* U *and other in* U'. *A bipartite graph is complete if each vertex of* U *is adjacent to all the vertices of* U'. *A* ***complete bipartite graph*** *with* $|U| = m$ *and* $|U'| = n$ *is denoted by* $K_{m,n}$. *The complete bipartite graph* $K_{1,n}$ *is called a* ***star***.

Definition 7. *Let G be a graph. The* ***complement*** *of G, denoted by $\overline{G}$ is defined as a graph with vertex set V and two vertices u, v are adjacent in $\overline{G}$ if they are not adjacent in G. $\overline{K_p}$ is the* ***totally disconnected*** *graph. $\overline{nK_2}$ is called the* ***cock-tail party graph*** *denoted by $CP(n)$. A graph G is* ***self-complementary*** *if $G = \overline{G}$.*

Definition 8. *The* ***degree matrix*** *of G, denoted by $\hat{D}$ is defined by $\hat{D} = [\hat{d}_{ij}]$ where*

$$\hat{d}_{ij} = \begin{cases} \deg(v_i)\,; \; i = j \\ 0; \; i \neq j \end{cases}$$

Definition 9. *Let G be a connected graph. The* ***distance*** *between the vertices u and v, denoted by $d(u,v)$ is the length of a shortest $u - v$ path. The* ***distance matrix*** *$\mathcal{D}$ of G is defined by $\mathcal{D} = [d_{ij}]$ where $d_{ij} = d(v_i, v_j)$; $i, \; j = 1, 2, \ldots, p$.*

Definition 10. *An* ***adjacency matrix*** *of G denoted by $A = A(G) = [a_{ij}]$ is a square matrix of order p where*

$$a_{ij} = \begin{cases} 1 \text{ if } v_i \text{ is adjacent to } v_j \\ 0 \text{ otherwise} \end{cases}$$

The ***characteristic polynomial*** *$|\lambda I - A|$ of A is called the characteristic polynomial of G and is denoted by $P_G(\lambda)$ or $P(G) = \sum_{i=1}^{p} a_i \lambda^{p-i}$. The* ***eigenvalues*** *of A, which are the zeros of $|\lambda I - A|$ are called the eigenvalues of G and form its* ***spectrum*** *denoted by spec(G). If the distinct eigenvalues of G are $\lambda_1, \; \lambda_2, \ldots, \lambda_m$ with multiplicities $t_1, \; t_2, \ldots, t_m$ respectively, then, spec(G) is written as*

$$\begin{pmatrix} \lambda_1 & \lambda_2 & \cdots\cdots & \lambda_m \\ t_1 & t_2 & & t_m \end{pmatrix} \text{ or } \left[\lambda_1^{t_1}, \lambda_2^{t_2}, \ldots\ldots, \lambda_m^{t_m}\right].$$

Note: Since the adjacency matrix is a real symmetric matrix, all of its eigenvalues are real and hence the eigenvalues can be ordered as $\lambda_1 \geqslant \lambda_2 \geqslant \ldots\ldots\ldots \geqslant \lambda_p$.

Also, rational eigenvalues are integers as the characteristic polynomial is monic.

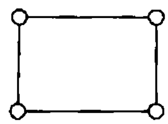


Figure 1.1: $G = C_4$

$$A(C_4) = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}, \ P(C_4) = \lambda^2(\lambda^2 - 4) \text{ and } spec(C_4) = [-2^1, 0^2, 2^1].$$

Note: Two isomorphic graphs have the same spectrum.

Definition 11. *Two non-isomorphic graphs G and H with $spec(G) = spec(H)$ are called* ***cospectral.***

Figure 1.2: Cospectral graphs with characteristic polynomial, $\lambda^3(\lambda^2 - 4)$.

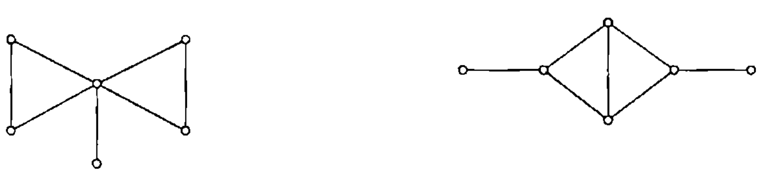


Figure 1.3: Cospectral connected graphs with characteristic polynomial, $\lambda^6 - 7\lambda^4 - 4\lambda^3 + 7\lambda^2 + 4\lambda - 1$.

Definition 12. *Let G be a graph with spec(G) = $\{\lambda_1,\ \lambda_2, \ldots\ldots, \lambda_p\}$. Then, the **energy** of G, denoted by $\mathcal{E}(G)$ is defined as* $\mathcal{E}(G) = \sum_{i=1}^{p} |\lambda_i|$.

Note: Cospectral graphs have the same energy.

Definition 13. *Two non-cospectral connected graphs G and H of the same order with $\mathcal{E}(G) = \mathcal{E}(H)$ are called **equienergetic graphs**.*

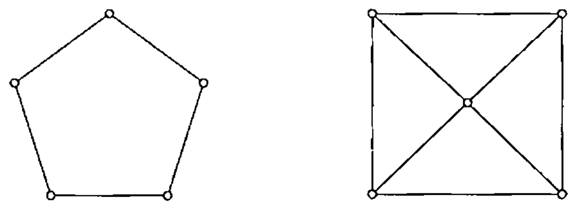


Figure 1.4: Two equienergetic graphs with energy $2(1+\sqrt{5})$.

Definition 14. *Let G be a (p, q) graph . The **line graph** of G, denoted by $L(G)$ is defined as a graph whose vertices are the edges of G and two vertices of $L(G)$ are adjacent if the corresponding edges are adjacent in G. The **iterated line graphs** of G are defined by $L^k(G) = L(L^{k-1}(G))$.*

Definition 15. *Let G be a (p, q) graph. The subdivision graph $S(G)$ of G is obtained from G by replacing each of its edges by a path of length 2.*

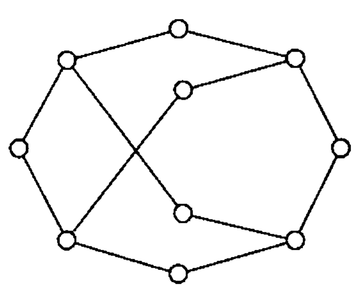


Figure 1.5: $S(K_4)$

Definition 16. *Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_p\}$. Take a set $U = \{u_1, u_2, \ldots, u_p\}$ of p vertices. Make u_i adjacent to all the vertices in $N(v_i)$ for each i, $i = 1$ to p. The resulting graph is called the* ***splitting graph*** *of G denoted by $splt(G)$.*

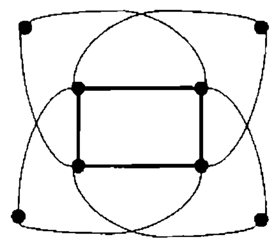


Figure 1.6: $splt(C_4)$.

Definition 17. *Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_p\}$. Take another set $U = \{u_1, u_2, \ldots, u_p\}$. Make u_i adjacent to all the vertices in $N(v_i)$ in G for each i and remove edges of G only. The resulting graph H is called the* ***duplication graph*** *of G denoted by DG.*

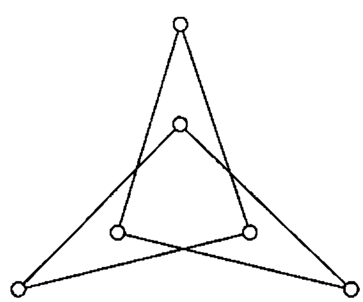


Figure 1.7: DC_3.

Definition 18. *Let $G = (V, E)$ and $H = (V', E')$ be two graphs. The* ***cartesian product*** *of G and H, denoted by $G \times H$ is defined as a graph with $V(G \times H) = V \times V'$ and two vertices (u, v) and (u', v') are adjacent if either $u = u'$ and v is adjacent to v' in H or u is adjacent to u' in G and $v = v'$.*

Definition 19. *The* ***tensor product*** *of G and H, denoted by $G \otimes H$ is defined as a graph with $V(G \otimes H) = V \times V'$ and two vertices (u, v) and (u', v') are adjacent if and only if u is adjacent to v in G and u' is adjacent to v' in H.*

Definition 20. *Let G and H be two graphs. Then, the* ***complete product(join)*** *of G and H, denoted by $G \nabla H$ is obtained by making every vertex of G adjacent to all the vertices of H.*

Definition 21. *Let $A = [a_{ij}]$ and $B = [b_{ij}]$ be two matrices of order $m \times n$ and $s \times t$ respectively. Then, their tensor product, $A \otimes B$ is obtained from A when every element a_{ij} is replaced by the block $a_{ij}B$ and is of order $ms \times nt$.*

Definition 22. *Let $\mathcal{B}$ be a set of binary $n-$tuples, $\mathcal{B} \subseteq \{0,1\}^n - \{(0,0,\ldots,0)\}$ such that for every $i = 1, 2, \ldots, n$ there exists $\beta \in \mathcal{B}$ with $\beta_i = 1$. The non-complete extended $p-$sum* ***(NEPS)*** *of graphs $G_1,\ G_2, \ldots, G_n$ with basis $\mathcal{B}$, denoted by NEPS $(G_1,\ G_2, \ldots, G_n, \mathcal{B})$, is the graph with the vertex set $V(G_1) \times V(G_2) \times \ldots \times V(G_n)$ in which two vertices $(u_1, u_2, \ldots, u_n)$ and $(v_1, v_2, \ldots, v_n)$ are adjacent if and only if there exists $\beta = (\beta_1, \beta_2, \ldots, \beta_n) \in \mathcal{B}$ such that u_i is adjacent to v_i in G_i whenever $\beta_i = 1$ and $u_i = v_i$ whenever $\beta_i = 0$.*

Note: When $n = 2$, the NEPS is the cartesian product of G_1 and G_2 for $\mathcal{B} = \{(1,0),(0,1)\}$ and the tensor product of G_1 and G_2 for $\mathcal{B} = \{(1,1)\}$.

Definition 23. *Let G be a (p, q) graph. The* ***incidence matrix*** *$R = [r_{ij}]$ is defined by*

$$r_{ij} = 1 \text{ if } v_i \text{ is incident with } e_j$$
$$= 0, \text{ otherwise.}$$

Definition 24. *A graph G is* **reciprocal** *if the reciprocal of each of its eigenvalue is also an eigenvalue of G.*

Definition 25. *Let G be a connected graph with distance matrix $\mathcal{D}$. Then, the* ***Wiener index*** *of G, denoted by $W(G)$ is defined as $W(G) = \frac{1}{2}\sum_{d\in\mathcal{D}} d$.*

Definition 26. *A graph G is* **integral** *if all of its eigenvalues are integers.*

Definition 27. *A graph G in which one vertex v is distinguished from the rest is a graph* **rooted** *at v.*

Definition 28. *A graph G is said to be a* **split graph** *if its vertex set can be partitioned into V_1 and V_2 such that V_1 induces a complete graph and V_2 induces a totally disconnected graph.*

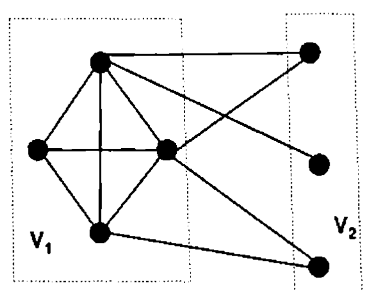


Figure 1.8: A split graph with vertex partition V_1 and V_2.

Definition 29. *Let G be a (p,q) graph with energy $\mathcal{E}$. Then, the Türker angles α, β and θ are given by*

$$\tan\alpha = \frac{Y}{p+\mathcal{E}}; \tan\beta = \frac{Y}{2q+\mathcal{E}} \text{ and } \tan\theta = \frac{Y}{\mathcal{E}} \text{ where } Y = \sqrt{2pq-\mathcal{E}^2}.$$

We shall now list some results used in this thesis.

Lemma 1.1. *[24] Let M, N, P and Q be matrices with M invertible. Let $S = \begin{bmatrix} M & N \\ P & Q \end{bmatrix}$. Then, $|S| = |M|\,|Q - PM^{-1}N|$ and if M and P commutes, then, $|S| = |MQ - PN|$ where the symbol $|.|$ denotes the determinant.*

Lemma 1.2. *[31] Let $A = \begin{bmatrix} A_0 & A_1 \\ A_1 & A_0 \end{bmatrix}$ be a 2×2 block symmetric matrix. Then, the eigenvalues of A are those of $A_0 + A_1$ together with those of $A_0 - A_1$.*

Lemma 1.3. *[24] Let G be an $r-$ regular graph on p vertices with an adjacency matrix A. Then, an adjacency matrix $\overline{A}$ of $\overline{G}$ is $\overline{A} = J - I - A$ where J and I are the all one square matrix and the identity matrix of order p respectively .*

Lemma 1.4. *[24] Let G be an $r-$ regular graph with an adjacency matrix A and incidence matrix R. Then, $RR^T = A + rI$.*

Lemma 1.5. *[24] Let G be a (p,q) graph with $spec(G) = \{\lambda_1, \lambda_2, \ldots, \lambda_p\}$. Then,*

1. $\sum_{i=1}^{p} \lambda_i = 0$, $\sum_{i=1}^{p} \lambda_i^2 = 2q$.
2. $\sum_{i=1}^{p} \lambda_i^3 = 6t$ *where t is the number of triangles in G.*
3. *If G is connected and $r-$ regular, then, r is the simple and the greatest eigenvalue of G.*

Lemma 1.6. *[24] Let G be a graph with an adjacency matrix A and $spec(G) = \{\lambda_1, \lambda_2, \ldots, \lambda_p\}$. Then, $\det A = \prod_{i=1}^{p} \lambda_i$. Also for any polynomial $P(x)$, $P(\lambda)$ is an eigenvalue of $P(A)$ and hence $\det P(A) = \prod_{i=1}^{p} P(\lambda_i)$.*

Lemma 1.7. *[24] Let G be a connected r-regular graph on p vertices with an adjacency matrix A having m distinct eigenvalues $\lambda_1 = r$, $\lambda_2, \ldots, \lambda_m$. Then, there exists a polynomial $Q(x) = p \times \frac{(x-\lambda_2)(x-\lambda_3)\ldots(x-\lambda_m)}{(r-\lambda_2)(r-\lambda_3)\ldots(r-\lambda_m)}$, such that $Q(A) = J$ so that $Q(r) = p$ and $Q(\lambda_i) = 0 \; \forall \lambda_i \neq r$.*

Lemma 1.8. *[24] Let G be a (p,q) graph with an adjacency matrix A and degree matrix $\hat{D}$. Then, the characteristic polynomial of $L(G)$ is given by*
$P_{L(G)}(\lambda - 2) = \lambda^{q-p} \left| \lambda I - A - \hat{D} \right|$.

Lemma 1.9. *[24] Let G be r_1- regular on p_1 vertices and H, r_2- regular on p_2 vertices. Then, $P(G \nabla H) = \frac{P(G)P(H)}{(\lambda - r_1)(\lambda - r_2)} \left[\lambda^2 - (r_1 + r_2)\lambda + r_1 r_2 - p_1 p_2\right]$.*

Lemma 1.10. *[86] Let G and H be two graphs rooted at u and v respectively.*

1. *Let F be the graph obtained by joining u and v by an edge. Then,*
   $P(F) = P(G)P(H-v) + P(G-u)P(H) - \lambda P(G-u)P(H-v)$.

2. *Let F' be the graph obtained by identifying u and v. Then,*
   $P(F') = P(G)P(H) - P(G-u)P(H-v)$.

Lemma 1.11. *[24]*

- $spec(K_p) = \begin{pmatrix} p-1 & -1 \\ 1 & p-1 \end{pmatrix}$.

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

- $spec(CP(n)) = \begin{pmatrix} 2n-2 & 0 & -2 \\ 1 & n & n-1 \end{pmatrix}$.

- $spec(C_n) = \begin{pmatrix} 2\cos\frac{2\pi i}{n} \\ 1 \end{pmatrix}$, $i = 1$ *to* n.

- $spec(P_n) = \begin{pmatrix} 2\cos\frac{2\pi i}{n+1} \\ 1 \end{pmatrix}$, $i = 1$ *to* n.

Lemma 1.12. *[24] Let G be an $r-$ regular graph with $spec(G) = \{r, \lambda_2, \ldots, \lambda_p\}$. Then, $spec(\overline{G}) = \{p-r-1, -1-\lambda_2, \ldots, -1-\lambda_p\}$.*

Lemma 1.13. *[24]Let A and B be two matrices and $F = A \otimes B$ be their tensor product. Then, $spec(F) = \{\lambda_i\mu_j / \lambda_i \in spec\,(A), \mu_j \in spec\,(B)\}$. In particular let G and H be two graphs of order p and p' respectively with $spec(G) = \{\lambda_i\}$, $i = 1$ to p and $spec(H) = \{\mu_j\}$, $j = 1$ to p'. Let $F = G \otimes H$, the tensor product of G and H. Then, $spec(F) = \{\lambda_i\,\mu_j\}$, $i = 1$ to p and $j = 1$ to p'.*

Lemma 1.14. *[24] Let G and H be two graphs of order p and p' respectively with $spec(G) = \{\lambda_i\}$, $i = 1$ to p and $spec(H) = \{\mu_j\}$, $j = 1$ to p'. Let $F = G \times H$, the cartesian product of G and H. Then, the $spec(F) = \{\lambda_i + \mu_j\}$, $i = 1$ to p, $j = 1$ to p'.*

Lemma 1.15. *[77] Let G be an $r-$ regular graph with $spec(G) = \{r, \lambda_2, ..., \lambda_p\}$. Then, $spec(L^2(G)) = \begin{pmatrix} 4r-6 & \lambda_i + 3r - 6 & 2r-6 & -2 \\ 1 & 1 & \frac{p(r-2)}{2} & \frac{pr(r-2)}{2} \end{pmatrix}$, $i = 2$ to p*

$\mathcal{E}(L^2(G)) = 2pr(r-2)$ and $\mathcal{E}(\overline{L^2(G)}) = (pr-4)(2r-3) - 2$.

New definitions

Definition 30. *Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_p\}$. Take another copy of G with the vertices labelled as $\{u_1, u_2, \ldots, u_p\}$ where u_i corresponds to v_i for each i. Make u_i adjacent to all the vertices in $N(v_i)$ in G, for each i. The resulting graph is called the* ***double graph*** *of G, denoted by D_2G.*

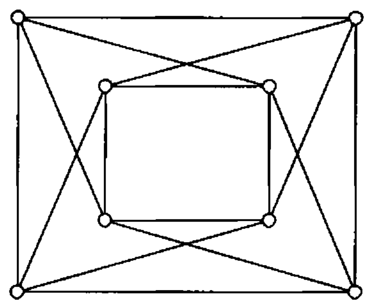


Figure 1.9: D_2C_4.

Definition 31. *Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_p\}$. Introduce a set of p isolated vertices $\{u_1, u_2, \ldots, u_p\}$ and make each u_i adjacent to all the vertices in $N(v_i)$ in G for each i. Introduce a set of k, $(k \geq 0)$ isolated vertices and make all of them adjacent to all the vertices of G only. The resulting graph is denoted by $\mathcal{G}_k$.*

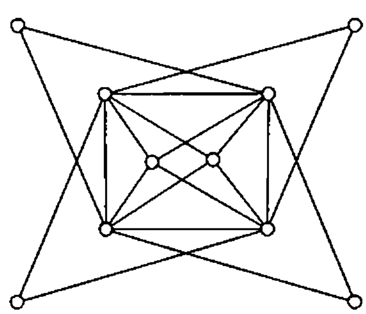


Figure 1.10: The graph $\mathcal{G}_2$ when $G = C_4$.

Note: When $k = 0$, $\mathcal{G}_0 = splt(G)$ (Definition 16).

Definition 32. *Let G be a (p,q) graph. The* ***complement of the incidence matrix*** *R, denoted by $\overline{R} = [\overline{r_{ij}}]$ is defined by*

$$\overline{r_{ij}} = 1 \text{ if } v_i \text{ is not incident with } e_j$$
$$= 0, \text{ otherwise.}$$

Definition 33. *Let G be a (p,q) graph. Corresponding to every edge e of G introduce a vertex and make it adjacent with all the vertices not incident with e in G. Delete the edges of G only. The resulting graph is called the* ***partial complement of subdivision graph*** *of G denoted by $\overline{S}(G)$.*

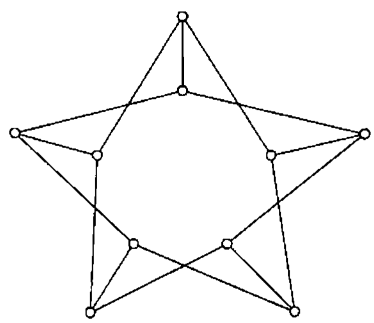


Figure 1.11: $\overline{S}(C_5)$

Definition 34. *A graph G is* ***partially reciprocal*** *if $\frac{-1}{\lambda} \in spec(G)$ for every $\lambda \in spec(G)$.*

Definition 35. *Let G be a (p,q) graph with $E(G) = \{e_1, e_2, ..., e_q\}$. Corresponding to every edge e_i introduce a set U_i^t of t isolated vertices and make every vertex in U_i^t adjacent to the vertices incident with e_i for each $i = 1, 2, ...q$. Now, delete edges of G only. The resulting graph is called the* ***$t-$ subdivision graph*** *of G denoted by $S(G)_t$.*

Note: $S(G)_1 = S(G)$ (Definition 15).

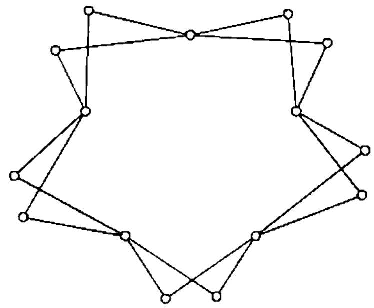


Figure 1.12: $S(C_5)_2$.

Definition 36. *Let G be a graph on $\{v_1, v_2, ..., v_p\}$. Corresponding to each v_i, introduce a set U_i^t of t isolated vertices. Make every vertex in U_i^t adjacent to all the vertices in $N(v_i)$ for each i. The resulting graph is called the* ***t*− splitting graph** *of G denoted by $splt(G)_t$.*

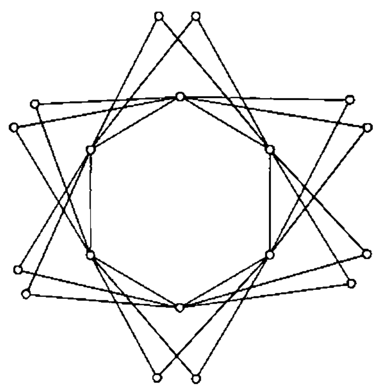


Figure 1.13: $splt(C_6)_2$.

Note: $splt(G)_1 = splt(G)$.

Definition 37. *Let G be a (p, q) graph with $E(G) = \{e_1, e_2, ..., e_q\}$. Corresponding to each e_i, introduce a set W_i^t of t isolated vertices. Make every vertex in W_i^t adjacent to the vertices incident with e_i for each i, $i = 1$ to q. The resulting graph is called the* ***t*− edge splitting graph** *of G denoted by $edsplt(G)_t$*

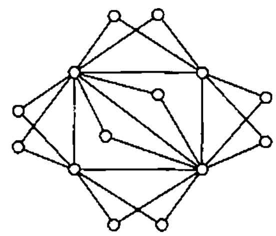


Figure 1.14: $edsplt(K_4 - e)_2$.

Definition 38. *Two non-isomorphic graphs G and H are Türker equivalent if they have the same set of values for the Türker angles α and β.*

1.2 List of symbols

$A(G)$ or A	-	the adjacency matrix of G.
C_n	-	the cycle on n vertices.
$CP(n)$	-	the cock-tail party graph on $2n$ vertices.
$\mathcal{D}$	-	distance matrix of G.
$\hat{D}$	-	the degree matrix of G.
DG	-	the duplication graph of G.
D_2G	-	the double graph of G.
$E(G)$ or E	-	the edge set of G.
$edsplt(G)_t$	-	the $t-$ edge splitting graph of G.
$\mathcal{E}$	-	the energy of G.
$G \times H$	-	the cartesian product of G and H.
$\{G\}^k$	-	the cartesian product of G, k times.
$G \otimes H$	-	the tensor product of G and H.
$G \nabla H$	-	the complete product(join) of G and H.
$\overline{G}$	-	the complement of G.

H_v^k	-	the graph obtained by identifying roots v in each of the k copies of H.
I	-	the identity matrix.
J	-	the square matrix with all entries equal to 1.
K_p	-	the complete graph on p vertices.
$K_{m,n}$	-	the complete bipartite graph.
$k *_G H$	-	the graph obtained by joining each of the roots in k copies of H to all the vertices of G.
$L(G)$	-	the line graph of G.
$N(v)$	-	the open neighborhood of v.
$N[v]$	-	the closed neighborhood of v.
$\overline{N(v)}$	-	$V(G) - N(v)$.
$\overline{N[v]}$	-	$V(G) - N[v]$.
p	-	the order of G.
$P(G)$	-	the characteristic polynomial of G.
P_n	-	the path on n vertices.
q	-	the size of G.
R	-	the incidence matrix.
$\overline{R}$	-	the complement of the incidence matrix.
$spec(G)$	-	the spectrum of G.
$S(G)$	-	the subdivision graph of G.
$\overline{S}(G)$	-	the partial complement of the subdivision graph.
$S(G)_t$	-	the $t-$ subdivision graph of G.
$splt(G)$	-	the splitting graph of G.
$splt(G)_t$	-	the $t-$ splitting graph of G.
$V(G)$ or V	-	the vertex set of G.

$W(G)$ - the Wiener index of G.

1.3 The spectrum and energy of graphs - A survey of results

As remarked earlier, the foundations of spectral graph theory were laid during the early 1950s by studying the relation between spectral and structural properties of graphs. The following are the fundamental results pertaining to spectra of graphs.

- **Sach's Theorem:** The coefficients of $P(G)$ are given by $a_i = \sum_H (-1)^{k(H)} 2^{c(H)}$ where the summation extends over all subgraphs H of G on i vertices whose components are either single edges or cycles, and where $k(H)$ and $c(H)$ denote, respectively, the number of components and cycles in H.

- **Perron-Frobenius Theorem:** If G is a connected graph with at least two vertices, then,

  (a) its largest eigenvalue λ_1 is a simple root of $P(G)$;

  (b) corresponding to the eigenvalue λ_1, there is an eigenvector x_1 all of whose coordinates are positive;

  (c) if λ is any other eigenvalue of G, then, $-\lambda_1 \leq \lambda < \lambda_1$;

  (d) the deletion of any edge of G decreases the largest eigenvalue.

- **Coulson - Rushbrooke Theorem:** The following statements are equivalent for a connected graph G:

  (a) G is a bipartite graph;

  (b) $\lambda_p = -\lambda_1$;

  (c) $\lambda_i = \lambda_{p+1-i}$, for $1 \leq i \leq \frac{p-1}{2}$;

  (d) $a_{2i-1} = 0$, for $1 \leq i \leq \frac{p+1}{2}$

  (e) $\sum\limits_{j=1}^{p} \lambda_j^{2i-1} = 0$, for all $i \geq 1$;

- **The Interlacing Theorem:** Let G be a graph with spectrum $\lambda_1 \geqslant \lambda_2 \geqslant \ldots\ldots \geqslant \lambda_p$ and let the spectrum of $G - v$ be $\mu_1 \geqslant \mu_2 \geqslant \ldots\ldots \geqslant \mu_{p-1}$. Then,

$$\lambda_1 \geqslant \mu_1 \geqslant \lambda_2 \geqslant \mu_2 \geqslant \ldots\ldots \geqslant \mu_{p-1} \geqslant \lambda_p \, .$$

The approximative treatment of non-saturated hydrocarbons introduced by E. Hückel [53] yields a graph theoretical model of the corresponding molecules in which eigenvalues of graphs represent the energy levels of certain electrons. The connection between Hückel's model of 1931 and the mathematical theory of graph spectra was recognized many years later in [25] and [38]. The calculation of the characteristic polynomial of a molecular graph plays an important role in the theory of graph spectra [6, 7, 78].

Formulae for the characteristic polynomials of various local modifications of a graph are discussed in [89] . One of the first results of this nature deals with the spectrum of the graph $G - u$. Also, the characteristic polynomial of the line graph, the subdivision graph, the total graph and others of a given graph are studied in detail in [24]. Let G and H be two graphs rooted at u and v respectively. In [86] the characteristic polynomials of graphs formed by identifying u and v and by joining u and v by an edge, are described.

In the fundamental paper on the energy of unsaturated hydrocarbons by Coulson [18], it was proved that the energy $\mathcal{E} = \frac{1}{\pi} \int\limits_{-\infty}^{\infty} [p - \lambda \frac{d}{d\lambda} \log P(G : i\lambda)] d\lambda$ where p is the number of vertices of the molecular graph. In 1971 B.J. McClelland [71] used the eigenvalues of the molecular graph to express its energy. In 1978 I.Gutman [39] generalized the concept of energy to all graphs and defined energy of a graph G, $\mathcal{E}(G)$ as the sum of the absolute values of its eigenvalues. The concept of graph energy is elaborated in detail in [43] and in [41, 67, 69, 100, 101, 102, 109, 110]. For a detailed survey on energy of graphs see [42].

In [39] I.Gutman conjectured that among all graphs of order p, the complete graph K_p has maximum energy. In [100] H.B. Walikar disproved Gutman's conjecture and produced graphs whose energy exceed that of K_p and called such graphs as hyperenergetic. Also, the energy of some graphs obtained by deleting a set of edges from K_p and $K_{m,n}$ is discussed in [101] and non-hyperenergetic graphs are studied in [102]. In [95] the energy of the NEPS of graphs is studied and proved that the energy of NEPS of graphs can be expressed as a function of the energies of basic graphs if and only if the NEPS corresponds to the tensor product of graphs.

J.H.Koolen and V.Moulton [62] obtained a sharp upperbound for the energy of graphs and in [63] they extended it to bipartite graphs. They proved that $\mathcal{E}(G) \leqslant \frac{2q}{p} + \sqrt{(p-1)\left(2q - 4\frac{q^2}{p^2}\right)}$ in [62] and $\mathcal{E}(G) \leqslant \frac{4q}{p} + \sqrt{(p-2)\left(2q - 8\frac{q^2}{p^2}\right)}$, for bipartite graphs G in [63]. An upperbound for energy in terms of p, q and the degrees of vertices is obtained in [113] as $\mathcal{E}(G) \leqslant \sqrt{\frac{\sum_{i=1}^{p} d_i^2}{p}} + \sqrt{(p-1)\left(2q - \frac{\sum_{i=1}^{p} d_i^2}{p}\right)}$ where d_i, $i = 1$ *to* p are the degrees of vertices of G. For a bipartite graph the above bound is improved to $\mathcal{E}(G) \leqslant 2\sqrt{\frac{\sum_{i=1}^{p} d_i^2}{p}} + \sqrt{(p-2)\left(2q - \frac{2\sum_{i=1}^{p} d_i^2}{p}\right)}$. In [109] an upperbound for $\mathcal{E}$ in terms of p, q and sum of the degrees of vertices adjacent to $v \in V(G)$ is obtained.

In [50] Y.Hou proved that S_n^3, $n \geq 6$, the graph obtained from the star graph $K_{1,n-1}$ by adding an edge, is the unique minimal energy graph among all unicyclic graphs with n vertices. It is proved that P_n^6, the graph obtained by making a vertex of C_6 adjacent with a terminal vertex of P_{n-6}, has the maximal energy among all connected unicyclic bipartite graphs on n vertices in [51]. A.Chen in [17] obtained the second and third minimum values of energies of unicyclic graphs and determined the corresponding graphs.

Let $\mathcal{T}_{n,d}$ denote the set of trees on n vertices and diameter d. In [111] W. Yan and L. Ye, determined the unique tree in $\mathcal{T}_{n,d}$ with minimal energy and in [115] the trees in $\mathcal{T}_{n,d}$ with second-minimal energy have been characterized. In [114] it has been proved that $\mathcal{E}(G) \geq \frac{2\sqrt{2\delta\Delta}}{2(\delta+\Delta)-1}\sqrt{2pq}$ for a quadrangle-free graph G on p vertices and q edges with minimum degree δ and maximum degree Δ.

R. Balakrishnan [4] conjectured that the complement of a cycle on n vertices is non-hyperenergetic for $n \geq 4$ and produced equienergetic graphs on p vertices $p \equiv 0(mod\ 4)$. In [94] D. Stevanović disproved the conjecture and constructed equienergetic graphs on p vertices, $p \equiv 0(mod\ 5)$ in [93]. H.S.Ramane et.al [77] obtained equienergetic pair of graphs within the family of iterated line graphs of regular graphs and proved that if G and H are two non-cospectral $r-$ regular graphs, $r \geq 3$ on p vertices then, $L^2(G)$ and $L^2(H)$ are equienergetic with energy $2pr(r-2)$. R.Bapat in [9] proved that the rational energy of a graph is always an even integer. Shparlinski [90] derived the energy of some circulant graphs.

Another field of interest in graph spectra is the search for graphs with specific pattern in their spectra. It is well known [24] in the theory of graph spectra that all connected graphs, except complete multipartite and complete graphs, have their second largest eigenvalue greater than 0. In [91] Smith found all connected graphs with $\lambda_1 \leq 2$ and proved that a connected graph has exactly one positive eigenvalue if and only if it is a complete multipartite graph. I.Gutman and D.M Cvetkovic studied the spectral structure of graphs having a maximal eigenvalue not greater than 2 in [26]. In [22, 23, 30] graphs with least eigenvalue -2 and those with least eigenvalue at least $-\sqrt{3}$ are studied in detail. M.Petrovċ in [75] obtained graphs with exactly one eigenvalue less than 1 and in [76] he obtained graphs whose second largest eigenvalue does not exceed $\sqrt{2}-1$. In [16]graphs whose second largest eigenvalue does not exceed $\frac{1}{3}$ and in [28] graphs whose second largest eigenvalue does not exceed $\frac{\sqrt{5}-1}{2}$ are obtained.

In [49] F. Harary and A.J. Schwenk posed the question 'Which graphs have integral spectra?'. In [21] the problem of cubic integral graphs is discussed and in [87] all the thirteen connected cubic integral graphs are listed. In [29] the construction of $4-$ regular integral graphs is described. M.Roitman in [81] obtained an interesting construction of an infinite family of integral graphs in the class of complete tripartite graphs K_{n_1,n_2,n_3}. In [105] some constructions on integral graphs were studied and integral graphs $K_p^t, K_{a,b}^t, K_{a,a,\ldots,a}^t$ were obtained by L.G.Wang. P.Hansen in [47] characterized integral split graphs obtained from the complete product of graphs. Some new integral graphs based on the study of bipartite semiregular graphs were obtained in [112] by Zhang. M.Lepovic in [64, 65, 66] obtained integral graphs which belong to the class $\overline{\alpha K_{a,b}}$, $\overline{\alpha K_a \cup \beta K_b}$ or $\overline{\alpha K_a \cup \beta K_{b,b}}$.

It is well known from the elementary spectral theory that the complement and the line graph of an integral graph are integral and several graph operations like the cartesian product, the tensor product etc when applied to integral graphs result in integral graphs [8].

The search for integral graphs pertaining to the class of trees began with X.L. Li in [68] and the first basic result regarding integral trees that 'no integral tree except K_2 has a perfect matching' was obtained in [108]. Recently in [103, 104, 106] L.G. Wang and X.L. Li have constructed integral trees with diameter $4, 6$ or 8. In [107] some more integral graphs pertaining to the class of complete $r-$partite and regular graphs are obtained.

Another class of graphs which recently received attention is that of reciprocal graphs. In [85] the three classes of reciprocal graphs obtained by attaching pendant vertices to all the vertices of a path, cycle and star are described. In[32] some more classes of reciprocal graphs which forms the skeleton graphs of the chemical molecules are described. In [10] reciprocal graphs are also referred to as graphs with property R and in [11] reciprocal trees are characterized.

The Wiener index W is the oldest molecular-graph-based structure descriptor. It is defined [43] as the sum of the distances of all the pairs of the vertices of the molecular graph G and in [73, 79] the chemical properties of this index is well described. In [70] the Wiener indices of some reciprocal graphs are obtained.

In the theory of conjugated molecules it has been established that the gross part of the total π-electron energy $\mathcal{E}_\pi$ - as computed within the HMO approximation - is determined only by the parameters p and q [43]. In order to express the fine molecular-structure-dependent differences in the behavior of the total $\pi-$ electron energy of isomeric alternate hydrocarbons L. Türker in [97] introduced the concept of 'angle of total $\pi-$ electron energy θ' defined as

$$\cos\theta = \frac{\mathcal{E}_\pi}{2\sqrt{pq}}$$

and two other related angles α and β connected by $\alpha + \beta = \theta$.

In [45] I.Gutman extended the definition of these angles to all graphs as

$$\cos\alpha = \frac{p+\mathcal{E}}{\sqrt{p}\sqrt{p+2\mathcal{E}+2q}},\ \cos\beta = \frac{\mathcal{E}+2q}{\sqrt{p+2\mathcal{E}+2q}\sqrt{2q}} \tag{1.1}$$

Setting $Y = \sqrt{2pq - \mathcal{E}^2}$ we get

$$\tan\alpha = \frac{Y}{p+\mathcal{E}};\tan\beta = \frac{Y}{2q+\mathcal{E}} \text{ and } \tan\theta = \frac{Y}{\mathcal{E}} \tag{1.2}$$

These angles α, β and θ are referred to as the Türker angles.

The Türker angle θ has proven to be a useful novel concept in the theory of total $\pi-$ electron energy and it has found numerous applications. The fundamental properties of θ, α and β are discussed in [40, 44, 45, 46, 98, 99]. Numerical calculation performed on a representative set of benzenoid hydrocarbons reveals that the dependence of the angles α and β on molecular structure is very similar, and that their ratio is almost constant ($\alpha/\beta = 1.564 \pm .015$).

1.4 Summary of the thesis

This thesis entitled **'Studies on the Spectrum and the Energy of Graphs'** is divided into 6 chapters including this introductory one.

The following are some of the results proved in the second chapter.

★ Let G be a graph with $spec(G) = \{\lambda_i\}$, $i = 1$ to p. Then, $spec(DG) = \begin{pmatrix} \lambda_i & -\lambda_i \\ 1 & 1 \end{pmatrix}$, $spec(D_2G) = \begin{pmatrix} 2\lambda_i & 0 \\ 1 & p \end{pmatrix}$, $i = 1$ *to* p and DG and D_2G are equienergetic.

★ Let G be a connected r-regular graph on p vertices and $\mathcal{G}_k$ be the graph as given in Definition 31. Then, $\mathcal{E}(\mathcal{G}_k) = \sqrt{5}\left[E(G) + \sqrt{r^2 + \frac{4}{5}pk} - r\right]$.

★ There exists a pair of equienergetic graphs for $p = 6,\ 14,\ 18$ and $p \geq 20$.

Let G be a graph. We apply the following constructions [33] on G which yield non-regular self-complementary graphs H_i, $i = 1$ *to* 4.

Construction 1. H_1 : *Replace each of the end vertices of* P_4 *by a copy of* G *and each of the internal vertices by a copy of* $\overline{G}$. *Join the vertices of these graphs by all possible edges whenever the corresponding vertices of* P_4 *are adjacent.*

Construction 2. H_2 : *Replace each of the end vertices of* P_4 *by a copy of* $\overline{G}$ *and each of the internal vertices by a copy of* G. *Join the vertices of these graphs by all possible edges whenever the corresponding vertices of* P_4 *are adjacent.*

Construction 3. H_3 : *Replace each of the end vertices of the non-regular self-complementary graph* F *on 5 vertices by a copy of* $\overline{G}$, *each of the vertices of degree 3 by a copy of* G *and the vertex of degree 2 by* K_1. *Join the vertices of these graphs by all possible edges whenever the corresponding vertices of* F *are adjacent.*

Construction 4. H_4 : *Consider the regular self-complementary graph* $C_5 = v_1v_2v_3v_4v_5v_1$. *Replace the vertices* v_1 *and* v_5 *by a copy of* $\overline{G}$, v_2 *and* v_4 *by a copy of* G *and* v_3 *by* K_1. *Join the vertices of these graphs by all possible edges whenever the corresponding vertices of* C_5 *are adjacent.*

★ Let G be an $r-$ regular connected graph on p vertices with $spec(G) = \{r, \lambda_2, \ldots\ldots, \lambda_p\}$ and H_1 be the self-complementary graph obtained by Construction 1. Then,

$$\mathcal{E}(H_1) = 2\left[\mathcal{E}(G) + \mathcal{E}(\overline{G}) - (p-1)\right] + \sqrt{(2p-1)^2 + 4\left\{(p-r)^2 + r\right\}} + \sqrt{1 + 4\left(p^2 + r + r^2\right)}.$$

★ Let G be an $r-$ regular connected graph on p vertices with $spec(G) = \{r, \lambda_2, \ldots\ldots, \lambda_p\}$ and H_2 be the self-complementary graph obtained by Construction 2. Then,

$$\mathcal{E}(H_2) = 2\left[\mathcal{E}(G) + \mathcal{E}(\overline{G}) - (p-1)\right] + \sqrt{(2p-1)^2 + 4\left\{(p-r)^2 + r\right\}} + \sqrt{1 + 4\left(p^2 + r + r^2\right)}$$

★ For every $p = 4k,\ k \geq 2$, there exists a pair of equienergetic self-complementary graphs.

★ Let H_3 be the self-complementary graph obtained from K_p by Construction 3. Then, $\mathcal{E}(H_3) = 2(p-1) + \sqrt{4p^2+1} + \sqrt{8p^2+4p+1}$.

★ Let H_4 be the self-complementary graph obtained from K_p by Construction 4. Then, $\mathcal{E}(H_4) = 2\left(2p-1\right) + \sqrt{4p+1} + \sqrt{8p^2-4p+1}$.

★ Let G be an $r-$ regular connected graph on p vertices with $spec(G) = \{r, \lambda_2, \ldots\ldots, \lambda_p\}$ and H_4 be the self-complementary graph obtained as in Construction 4. Then, $\mathcal{E}(H_4) = 2\left[\mathcal{E}(G) + \mathcal{E}(\overline{G}) - (p-1)\right] + \sqrt{1 + 4\left(p^2 + r + r^2\right)} + T$ where T is the sum of absolute values of roots of the cubic $x^3 - (2p-1)\,x^2 - \left[p^2 - 2p\,(r-1) + r\,(r+1)\right]x + 2p\,(2p-r-1) = 0$.

★ For every $p = 24t + 1,\ t \geq 3$, there exists a pair of equienergetic self-complementary graphs.

★ Let G be an $r-$ regular connected graph on p vertices, $p \geq 3$ and H_1, the graph obtained from G by Construction 1. Then, $\mathcal{E}(L(H_1)) = 4p(4p-5)$.

★ Let G be an $r-$ regular graph on p vertices with $r \geqslant 2(k+1)$. Then, for any graph F on n vertices whose spectrum is contained in $[-2k, 2k]$, $\mathcal{E}\left[\left\{L^2(G)\right\}^k \times F\right] = \frac{nk}{2^{k-2}}\left[pr(r-2)\right]^k$.

★ Let m and k be positive integers with $m \geq 2k$. Then, for any graph G on p vertices whose spectrum is contained in $[-k, k]$,
$\mathcal{E}\left[\{K_m\}^k \times G\right] = 2pk(m-1)^k.$

★ Let G be an $r-$regular graph on p vertices, $p \geq 4$ with $spec(G) = \{r, \lambda_2, ..., \lambda_p\}$. Then, $\mathcal{E}(L[G\nabla\overline{G}]) = 2p(3p-5)$.

In the third chapter we obtain the eigenvalues of some non-regular graphs and their complements, the energy of some non-regular graphs and energy of two classes of regular graphs.

Some results in this chapter are:

- Let G be a connected $r-$ regular (p, q) graph with an adjacency matrix A and $spec(G) = \{r, \lambda_2, \lambda_3, ..., \lambda_p\}$.
  Then, $spec(\overline{S}(G)) = \begin{pmatrix} \pm\sqrt{p(q-2r)+2r} & \pm\sqrt{\lambda_i + r} & 0 \\ 1 & 1 & q-p \end{pmatrix}, i = 2 \; to \; p.$

- $$\mathcal{E}\left(\overline{S}\left(C_p\right)\right) = \begin{cases} 2\left(p - 4 + 2\cot\frac{\pi}{2p}\right), p \equiv 0(mod\ 2) \\ \\ 2\left(p - 4 + 2\mathrm{cosec}\frac{\pi}{2p}\right), p \equiv 1(mod\ 2) \end{cases}$$

- $$\mathcal{E}\left(\overline{C_p}\right) = \begin{cases} 2\left(\frac{2p-9}{3} + \sqrt{3}\cot\frac{\pi}{p}\right); p \equiv 0(mod\ 3) \\ \\ 2\left(\frac{2p-8}{3} + \frac{2\sin\frac{\pi}{3}\left(1-\frac{1}{p}\right)}{\sin\frac{\pi}{p}}\right); p \equiv 1(mod\ 3) \\ \\ 2\left(\frac{2p-10}{3} + \frac{2\sin\frac{\pi}{3}\left(1+\frac{1}{p}\right)}{\sin\frac{\pi}{p}}\right); p \equiv 2(mod\ 3) \end{cases}$$

In the fourth chapter we consider some operations on graphs, which are described as follows.

Operation 1. *Attach a pendant vertex to each vertex of G. The resulting graph is called the pendant join graph of G.*

Operation 2. *The splitting graph of G (Definition 16).*

Operation 3. *In addition to G introduce two sets of p isolated vertices $U = \{u_i\}$ and $W = \{w_i\}$ corresponding to $V = \{v_i\}$, $i = 1$ to p. Make u_i and w_i adjacent to all the vertices in $N(v_i)$ and then, w_i to the vertices in U corresponding to the neighbors of v_i in G for each $i = 1$ to p. The resulting graph is called the double splitting graph of G.*

Operation 4. *In addition to G introduce two more copies of G on $U = \{u_i\}$ and $W = \{w_i\}$ corresponding to $V = \{v_i\}$, $i = 1$ to p. Make u_i adjacent to all the vertices in $N(v_i)$ and then, w_i to u_i for each $i = 1$ to p. The resulting graph is called the composition graph of G.*

Operation 5. *In addition to G introduce two more copies of G on $U = \{u_i\}$ and $W = \{w_i\}$ corresponding to $V = \{v_i\}$, $i = 1$ to p. Make w_i adjacent to all the vertices in $N(v_i)$ and vertices in U corresponding to the neighbors of v_i in G for each $i = 1$ to p.*

Using these operations we construct some new classes of reciprocal graphs. We derive the following results in this chapter.

- ✠ The pendant join graph of a graph G is reciprocal if and only if G is bipartite.
- ✠ The splitting graph of G is reciprocal if and only if G is partially reciprocal.
- ✠ Let G be a reciprocal graph. Then, the double splitting graph and the composition graph of G are reciprocal if and only if G is bipartite.
- ✠ Let G be a (p, q) reciprocal graph. Then, $\mathcal{E}(G) \leq \sqrt{\frac{p(2q+p)}{2}}$ and the bound is best possible for $G = tK_2$ and tP_4.
- ✠ There exists a pair of equienergetic reciprocal graphs on every $p \equiv 0(mod\ 12)$, $p \geq 36$ and $p \equiv 0(mod\ 16)$, $p \geq 48$.
- ✠ Let G be a graph with Wiener index $W(G)$. Let H be the pendant join graph of G. Then, $W(H) = 4W(G) + p(2p - 1)$.
- ✠ Let G be a triangle free (p, q) graph and H, be its splitting graph. Then, $W(H) = 4W(G) + 2(p + q)$.
- ✠ Let G be a triangle free (p, q) graph and H, be its composition graph. Then, $W(H) = 9W(G) + 2p^2 + 4p$.
- ✠ Let G be a triangle free (p, q) graph and H be its double splitting graph. Then, $W(H) = 9W(G) + 4q + 6p$.

In the fifth chapter using the first two of the results listed below, some new integral graphs have been constructed. Some new integral graphs belonging to the family of split graphs have also been obtained.

- The characteristic polynomial of H_v^k is given by
  $P(H_v^k) = [P(H-v)]^{k-1}[kP(H) - (k-1)\lambda P(H-v)]$.

- Let G be an $r-$ regular graph on p vertices and H be rooted at v. Then,

$$P\left(F_k^t\right) = \frac{P(G)}{(\lambda - r)}\lambda^{k-(t+1)}[P(H)]^{t-1}$$
$$\times [P(H)\{\lambda(\lambda - r) - p(k-t)\} - tp\lambda P(H-v)].$$

- For every $p \equiv 0(mod\ 4)$, there exists a pair of equienergetic integral graphs.

The sixth chapter deals with some classes of Türker equivalent graphs. The results obtained are:

★ Let $\mathcal{G} = \{G/\text{G is an } r \geq 3 \text{ regular graph}\}$. Let $\mathcal{F}_k = \{L^k[G]/\text{G} \in \mathcal{G}\}$. Then, for each $k \geq 2$, the family $\mathcal{F}_k$ is Türker equivalent.

★ Let G be any graph. Let $\mathcal{D}_G = \bigcup\limits_k D^k G$. Then, the family $\mathcal{D}_G$ is Türker equivalent.

★ Let $\mathcal{G} = \{G/G \text{ is an } r \geq 3 \text{ regular graph}\}$, $\mathcal{H}_k = \{L^k(G),\ k \geq 2/G \in \mathcal{G}\}$ and $\mathcal{F}_k = \{F = H_1 \otimes H_2\ /H_1 \text{ and } H_2 \in \mathcal{H}_k\}$. Then, for each k,the family $\mathcal{F}_k$ is Türker equivalent.

★ Let G be an $r-$ regular graph on p vertices. Let $\mathcal{F} = \{L^k(G) \otimes K_n\}$. Then, for each n and k the family $\mathcal{F}$ is Türker equivalent.

★ Let G be an $r-$ regular graph with $r \geq 4$ on p vertices. Then, the family $L^k(G) \times C_n$ is Türker equivalent for each k.

★ Let $\mathcal{H}_k = \left\{L^k(G)/G \text{ is an } r \text{ regular graph}\right\}$ and $\mathcal{F}_k = \{splt(H_k)/\ H_k \in \mathcal{H}_k\}$. Then, for each k, the family $\mathcal{F}_k$ is Türker equivalent.

★ Let $\mathcal{H}_k = \left\{D_2\left[L^k(G)\right]/G \text{ is } r \geqslant 3 \text{ regular graph}\right\}$. Then, for each k the family $\mathcal{H}_k$ is Türker equivalent.

In this chapter some operations on graphs and resulting Türker equivalent graphs are also discussed.

Some of the results of this thesis are included in [54] to [59]. We conclude the thesis with some suggestions for further study and a bibliography.

1.5 List of publications

List of papers presented

- Presented a paper entitled 'Energies of cross product of graphs' in the 20th Annual Conference of the Ramanujan Mathematical Society held at University of Calicut during 27 - 30 July 2005.
- Presented a paper entitled 'Some integral graphs' in the poster session of the International Conference in Discrete Mathematics held at IISc Bangalore during 15 - 18 December 2006.

List of publications

- G. Indulal, A. Vijayakumar, *On a pair of equienergetic graphs*, MATCH Commun. Math. Comput. Chem., **55**(2006), 83 - 90.[54]
- G. Indulal, A. Vijayakumar, *Energies of some non-regular graphs*, J. Math. Chem., (to appear). Available online at *www.springerlink.com/content/y5x275l582386qn3* [55]
- G. Indulal, A. Vijayakumar, *Equienergetic self-complementary graphs*, Czechoslovak Math. J.(to appear).[56]
- G. Indulal, A. Vijayakumar, *Some new integral graphs*, Applicable Analysis and Discrete Mathematics, (to appear). Available online at http://pefmath.etf.bg.ac.yu/accepted/rad574.pdf [57]
- G. Indulal, A. Vijayakumar, *Türker equivalent graphs*, (Communicated).[58]
- G. Indulal, A. Vijayakumar, *Reciprocal graphs*, (Communicated).[59]

Chapter 2

Equienergetic graphs

In this chapter we construct

- Pair of equienergetic graphs for $p = 6,\ 14,\ 18$ and $p \geqslant 20$.
- Pair of equienergetic self-complementary graphs for every $p = 4k,\ k \geq 2$ and $p = 24t + 1,\ t \geq 3$.
- Pairs of equienergetic graphs using some other operations on graphs.

Some results of this chapter are included in the following papers.

- On a pair of equienergetic graphs, MATCH Commun. Math. Comput. Chem., **55**(2006), 83 - 90.
- Energies of some non-regular graphs, J. Math. Chem., (to appear).
- Equienergetic self-complementary graphs, Czechoslovak Math. J.(to appear)

2.1 New equienergetic graphs

Lemma 2.1. *Let G be a graph with $spec(G) = \{\lambda_1, \lambda_2, \dots, \lambda_p\}$ and an adjacency matrix A. Then, $spec(DG) = \begin{pmatrix} \lambda_i & -\lambda_i \\ 1 & 1 \end{pmatrix}$, $spec(D_2G) = \begin{pmatrix} 2\lambda_i & 0 \\ 1 & p \end{pmatrix}$, $i = 1$ to p and DG and D_2G are equienergetic.*

Proof. By Definition 17, the adjacency matrix of DG can be written as

$$A(DG) = \begin{bmatrix} 0 & A \\ A & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes A\,.$$

Then, by Lemma 1.13, $spec(DG) = \begin{pmatrix} \lambda_i & -\lambda_i \\ 1 & 1 \end{pmatrix}, i = \ 1 \ to \ p.$

Also by Definition 30, the adjacency matrix of D_2G can be written as

$$A(D_2G) = \begin{bmatrix} A & A \\ A & A \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \otimes A\,.$$

Then, by Lemma 1.13, $spec(D_2G) = \begin{pmatrix} 2\lambda_i & 0 \\ 1 & p \end{pmatrix}, i = \ 1 \ to \ p$

as $spec\left(\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\right) = \begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix}$.

Thus, by the definition of energy, DG and D_2G are equienergetic. □

Theorem 2.1. *Let G be a connected $r-$ regular graph on p vertices with $spec(G) = \{r, \lambda_2, \ldots, \lambda_p\}$. Let $\mathcal{G}_k$ be the graph as in Definition 31.*
Then, $\mathcal{E}(\mathcal{G}_k) = \sqrt{5}\left[\mathcal{E}(G) + \sqrt{r^2 + \frac{4}{5}pk} - r\right]$.

Proof. Let A be an adjacency matrix of G and J be the all one matrix. Then, the adjacency matrix of $\mathcal{G}_k$ can be written as

$$\begin{bmatrix} A & A & J_{p\times k} \\ A & 0 & 0 \\ J_{k\times p} & 0 & 0 \end{bmatrix}.$$

The characteristic equation of $\mathcal{G}_k$ is

$$\begin{vmatrix} \lambda I - A & -A & -J_{p\times k} \\ -A & \lambda I & 0 \\ -J_{k\times p} & 0 & \lambda I_k \end{vmatrix} = 0 \tag{2.1}$$

Now, L.H.S of Equation (2.1) is

$$\begin{vmatrix} \lambda I_k & 0 & -J_{k\times p} \\ 0 & \lambda I & -A \\ -J_{p\times k} & -A & \lambda I - A \end{vmatrix}$$
$$= \lambda^k \left| \begin{bmatrix} \lambda I & -A \\ -A & \lambda I - A \end{bmatrix} - \begin{bmatrix} 0 \\ -J_{p\times k} \end{bmatrix} \frac{I}{\lambda} \begin{bmatrix} 0 & -J_{k\times p} \end{bmatrix} \right|$$

$$= \lambda^{k-2p} \begin{vmatrix} \lambda^2 I & -A\lambda \\ -A\lambda & \lambda^2 I - A\lambda - kJ \end{vmatrix}$$

$$= \lambda^k \left| \lambda^2 I - A\lambda - kJ - A^2 \right|$$

Therefore the Equation (2.1) implies $[\lambda^2 - \lambda_i\lambda - kQ(\lambda_i) - \lambda_i^2] = 0$, by Lemmas 1.6 and 1.7 .

$$\text{Thus, } spec(\mathcal{G}_k) = \begin{pmatrix} \frac{r \pm \sqrt{5r^2+4pk}}{2} & \left(\frac{1\pm\sqrt{5}}{2}\right)\lambda_i & 0 \\ 1 & 1 & k \end{pmatrix}, i = 2 \ to \ p.$$

and $\mathcal{E}(\mathcal{G}_k) = \sqrt{5}\left[\mathcal{E}(G) + \sqrt{r^2 + \frac{4}{5}pk} - r\right]$. □

We shall now discuss the problem of constructing pairs of equienergetic graphs on p vertices, by analyzing the various cases.

Theorem 2.2. *There exists a pair of equienergetic graphs for* $p = 6, 14, 18$ *and* $p \geq 20$.

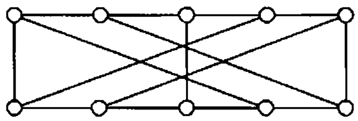
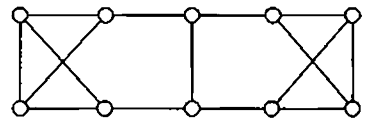
Proof.

Case 1. ***p= 6, 14, 18.***

Consider $G = C_3, C_7$ and C_9 respectively. Let $G_1 = DG$ and $G_2 = D_2G$ for each G. Then, both G_1 and G_2 are connected graphs on 6, 14, and 18 vertices, respectively and by Lemma 2.1, $\mathcal{E}(G_1) = \mathcal{E}(G_2) = 2\mathcal{E}(G)$.

Case 2. $p \geq 20$

The following cubic graphs G_1 and G_2 on 10 vertices are equienergetic with energy $11 + \sqrt{17}$ [24].

Then, by Theorem 2.1, the graphs $\mathcal{G}_k$ and $\mathcal{G}'_k$ obtained from these graphs are equienergetic on $20+k$, $k \geq 0$ vertices with energy $\sqrt{5}\left[8+\sqrt{17}+\sqrt{9+8k}\right]$. Hence the theorem. □

2.2 Equienergetic self-complementary graphs

In this section, we construct a pair of equienergetic self-complementary graphs, for $p = 4k$, $k \geq 2$ and $p = 24t + 1$, $t \geq 3$. Let G be a graph. Then, the following constructions [33] yield self-complementary graphs H_i, $i = 1$ to 4.

Construction 1. H_1 : *Replace each of the end vertices of* P_4 *by a copy of* G *and each of the internal vertices by a copy of* $\overline{G}$. *Join the vertices of these graphs by all possible edges whenever the corresponding vertices of* P_4 *are adjacent.*

Construction 2. H_2 : *Replace each of the end vertices of* P_4 *by a copy of* $\overline{G}$ *and each of the internal vertices by a copy of* G. *Join the vertices of these graphs by all possible edges whenever the corresponding vertices of* P_4 *are adjacent.*

Construction 3. H_3 : *Replace each of the end vertices of the non-regular self-complementary graph* F *on 5 vertices by a copy of* $\overline{G}$, *each of the vertices of degree 3 by a copy of* G *and the vertex of degree 2 by* K_1. *Join the vertices of these graphs by all possible edges whenever the corresponding vertices of* F *are adjacent.*

Construction 4. H_4 : *Consider the regular self-complementary graph* $C_5 = v_1v_2v_3v_4v_5v_1$, *the cycle on 5 vertices. Replace the vertices* v_1 *and* v_5 *by a copy of* $\overline{G}$, v_2 *and* v_4 *by a copy of* G *and* v_3 *by* K_1. *Join the vertices of these graphs by all possible edges whenever the corresponding vertices of* C_5 *are adjacent.*

Note: For all non-self-complementary graphs G, Constructions 1 and 2 yield non-isomorphic graphs and for any graph G, $H_1(G) = H_2(\overline{G})$.

Theorem 2.3. *Let* G *be an* $r-$ *regular connected graph with* $spec(G) = \{r, \lambda_2, \dots, \lambda_p\}$ *and* H_1 *be the self-complementary graph obtained by Construction 1. Then,*

$$\begin{aligned}\mathcal{E}(H_1) =& 2\left[\mathcal{E}(G) + \mathcal{E}(\overline{G}) - (p-1)\right] + \sqrt{(2p-1)^2 + 4\left\{(p-r)^2 + r\right\}} \\ &+ \sqrt{1 + 4\left(p^2 + r + r^2\right)}\end{aligned}$$

Proof. The adjacency matrix of H_1 can be written as $\begin{bmatrix} A & J & 0 & 0 \\ J & \overline{A} & J & 0 \\ 0 & J & \overline{A} & J \\ 0 & 0 & J & A \end{bmatrix}$, so that the characteristic equation of H_1 is

$$\begin{vmatrix} \lambda I - A & -J & 0 & 0 \\ -J & \lambda I - \overline{A} & -J & 0 \\ 0 & -J & \lambda I - \overline{A} & -J \\ 0 & 0 & -J & \lambda I - A \end{vmatrix} = 0.$$

That is

$$\begin{vmatrix} -J & \lambda I - \overline{A} & 0 & -J \\ \lambda I - \overline{A} & -J & -J & 0 \\ -J & 0 & \lambda I - A & 0 \\ 0 & -J & 0 & \lambda I - A \end{vmatrix} = 0,$$

by a sequence of elementary transformations.

But, the last expression by virtue of Lemma 1.1 is

$$\left| J^2(\lambda I - A)^2 - \left[(\lambda I - A)\left(\lambda I - \overline{A}\right) - J^2\right]^2 \right| = 0 \text{ and so}$$

$$\prod_{i=1}^{p} \left\{ \langle Q(\lambda_i)\rangle^2 (\lambda - \lambda_i)^2 - \left[(\lambda - \lambda_i)(\lambda - Q(\lambda_i) + 1 + \lambda_i) - \langle Q(\lambda_i)\rangle^2\right]^2 \right\} = 0$$

by Lemmas 1.6 and 1.7. Now, corresponding to the eigenvalue r of G, the eigenvalues of H_1 are given by

$$p^2(\lambda - r)^2 - \left[(\lambda - r)(\lambda - p + 1 + r) - p^2\right]^2 = 0 \text{ by Lemmas 1.6 and 1.7.}$$

That is $\left[\lambda^2 + \lambda - (r^2 + r + p^2)\right]\left[\lambda^2 - (2p-1)\lambda - \left\{(p-r)^2 + r\right\}\right] = 0$.

So $\lambda = \dfrac{-1 \pm \sqrt{1 + 4(p^2 + r + r^2)}}{2}; \dfrac{2p - 1 \pm \sqrt{(2p-1)^2 + 4\left\{(p-r)^2 + r\right\}}}{2}$.

The remaining eigenvalues of H_1 satisfy $\prod_{i=2}^{p} \left[(\lambda - \lambda_i)(\lambda + 1 + \lambda_i)\right]^2 = 0$. Hence,

$$spec(H_1) = \begin{pmatrix} \frac{-1 \pm \sqrt{1+4(p^2+r+r^2)}}{2} & \frac{2p-1 \pm \sqrt{(2p-1)^2 + 4\left\{(p-r)^2 + r\right\}}}{2} & \lambda_i & -1 - \lambda_i \\ 1 & 1 & 2 & 2 \end{pmatrix},$$

$i = 2$ to p.

Now, the expression for $\mathcal{E}(H_1)$ follows. □

Theorem 2.4. *Let G be an $r-$ regular connected graph with $spec(G) = \{r, \lambda_2, \dots, \lambda_p\}$ and H_2 be the self-complementary graph obtained by Construction 2. Then,*

$$\mathcal{E}(H_2) = 2\left[\mathcal{E}(G) + \mathcal{E}(\overline{G}) - (p-1)\right] + \sqrt{(2p-1)^2 + 4\left\{(p-r)^2 + r\right\}} + \sqrt{1 + 4\left(p^2 + r + r^2\right)}$$

Proof. The adjacency matrix of H_2 can be written as $\begin{bmatrix} \overline{A} & J & 0 & 0 \\ J & A & J & 0 \\ 0 & J & A & J \\ 0 & 0 & J & \overline{A} \end{bmatrix}$. By a similar computation as in Theorem 2.3 in which A is replaced by $\overline{A}$, we get the characteristic polynomial of H_2 as

$$\prod_{i=1}^{p} \left\{ \left(Q(\lambda_i)\right)^2 \left(\lambda - Q(\lambda_i) + \lambda_i + 1\right)^2 - \left[\left(\lambda - \lambda_i\right)\left(\lambda - Q(\lambda_i) + 1 + \lambda_i\right) - \left(Q(\lambda_i)\right)^2\right]^2 \right\},$$

by Lemmas 1.6, 1.1 and 1.7. Hence

$$spec(H_2) = \begin{pmatrix} \frac{2p-1 \pm \sqrt{1+4(p^2+r+r^2)}}{2} & \frac{-1 \pm \sqrt{(2p-1)^2 + 4\left\{(p-r)^2 + r\right\}}}{2} & \lambda_i & -1-\lambda_i \\ 1 & 1 & 2 & 2 \end{pmatrix},$$

$i = 2$ to p .

Thus, the theorem follows. $\square$

Corollary 2.1.

1. *If $G = K_p$, then, $\mathcal{E}(H_1) = \mathcal{E}(H_2) = 2(p-1) + \sqrt{1+4p^2} + \sqrt{8p^2 - 4p + 1}$.*

2. *If $G = K_{n,n}$, then, $p = 2n$ and $\mathcal{E}(H_1) = \mathcal{E}(H_2) = 2(2p-3) + \sqrt{5p^2 - 2p + 1} + \sqrt{5p^2 + 2p + 1}$.*

Theorem 2.5. *For every $p = 4k$, $k \geq 2$, there exists a pair of equienergetic self-complementary graphs.*

Proof. Let H_1 and H_2 be the self-complementary graphs obtained from K_k by Constructions 1 and 2 respectively. Then, by Theorems 2.3 and 2.4, they are equienergetic on $p = 4k$ vertices. □

Illustration:

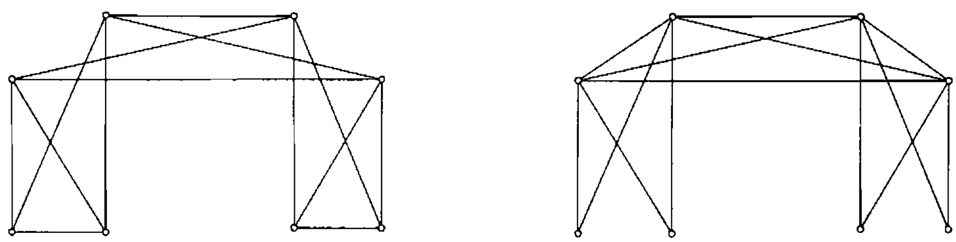


Figure 2.1: Equienergetic self-complementary graphs on 8 vertices with energy $7 + \sqrt{17}$.

Theorem 2.6. *Let H_3 be the self-complementary graph obtained from K_p by Construction 3. Then, $\mathcal{E}(H_3) = 2(p-1) + \sqrt{4p^2+1} + \sqrt{8p^2+4p+1}$.*

Proof. Let A be an adjacency matrix of K_p. Then, the adjacency matrix of H_3 can be written as

$$\begin{bmatrix} \overline{A} & J & 0_{p\times 1} & 0 & 0 \\ J & A & J_{p\times 1} & J & 0 \\ 0_{1\times p} & J_{1\times p} & 0 & J_{1\times p} & 0 \\ 0 & J & J_{p\times 1} & A & J \\ 0 & 0 & 0 & J & \overline{A} \end{bmatrix}.$$

Now, after a sequence of elementary transformations applied to the rows and columns and by Lemma 1.1, the characteristic equation of H_3 is

$$\frac{1}{\lambda^{2p-1}} \left| \left[\{\lambda(\lambda I - A) - J\} (\lambda I - \overline{A}) - \lambda J^2 \right]^2 - \left[(\lambda+1)(\lambda I - \overline{A}) J \right]^2 \right| = 0.$$

Since $G = K_p$ is connected and regular, by Lemmas 1.6 and 1.7, the characteristic equation of H_3 is

$$\lambda^{2p-1}(\lambda+1)^{2p-2}(\lambda^2+\lambda-p^2)\left[\lambda^2-(2p-1)\lambda-p(p+2)\right]=0.$$

So, $spec(H_3) = \begin{pmatrix} \frac{-1\pm\sqrt{4p^2+1}}{2} & \frac{2p-1\pm\sqrt{8p^2+4p+1}}{2} & -1 & 0 \\ 1 & 1 & 2p-2 & 2p-1 \end{pmatrix}$. Hence the theorem. $\square$

Theorem 2.7. *Let H_4 be the self-complementary graph obtained from K_p by Construction 4. Then, $\mathcal{E}(H_4) = 2(2p-1) + \sqrt{4p+1} + \sqrt{8p^2-4p+1}$.*

Proof. Let A be an adjacency matrix of K_p. Then, the adjacency matrix of H_4 can be written as

$$\begin{bmatrix} \overline{A} & J & 0_{p\times 1} & 0 & J \\ J & A & J_{p\times 1} & 0 & 0 \\ 0_{1\times p} & J_{1\times p} & 0_{1\times 1} & J_{1\times p} & 0 \\ 0 & 0 & J_{p\times 1} & A & J \\ J & 0 & 0 & J & \overline{A} \end{bmatrix}$$

Now, after a sequence of elementary transformations applied to the rows and columns and by Lemma 1.1, the characteristic equation of H_4 is

$$\frac{1}{\lambda^{2p-1}}\left|\begin{matrix} \left[\{\lambda(\lambda I-A)-J\}^2+(\lambda-1)J^2\right]\left[(\lambda-1)J^2+\left(\lambda I-\overline{A}\right)^2\right] \\ -\lambda J^2\left[\lambda(\lambda I-A)-J+\lambda I-\overline{A}\right]^2 \end{matrix}\right| = 0$$

Since $G = K_p$ is connected and regular, by Lemmas 1.6 and 1.7 the characteristic equation of H_4 is

$$\lambda^{(2p-2)}(\lambda+1)^{(2p-2)}(\lambda-2p)\left(\lambda^2+\lambda-p\right)\left(\lambda^2+\lambda-2p^2+p\right)=0.$$

Hence, $spec(H_4) = \begin{pmatrix} 2p & \frac{-1\pm\sqrt{4p+1}}{2} & \frac{2p-1\pm\sqrt{8p^2-4p+1}}{2} & -1 & 0 \\ 1 & 1 & 1 & 2p-2 & 2p-2 \end{pmatrix}$.

Now, the expression for $\mathcal{E}(H_4)$ follows.

□

Corollary 2.2. *Let G be a connected $r-$ regular graph and H_4 be the self-complementary graph obtained by Construction 4. Then,*

$$\mathcal{E}(H_4) = 2\left[\mathcal{E}(G) + \mathcal{E}(\overline{G}) - (p-1)\right] + \sqrt{1 + 4\left(p^2 + r + r^2\right)} + T$$

where T is the sum of absolute values of roots of the cubic

$x^3 - (2p-1)\,x^2 - \left[p^2 - 2p\,(r-1) + r\,(r+1)\right]x + 2p\,(2p-r-1) = 0.$

Lemma 2.2. *There exists a pair of non-cospectral cubic graphs on $2t$ vertices, for every $t \geq 3$.*

Proof. Let G_1 and G_2 be the non-cospectral cubic graphs on six vertices labelled as $\{v_j\}$ and $\{u_j\}$, $j = 1$ to 6 respectively.

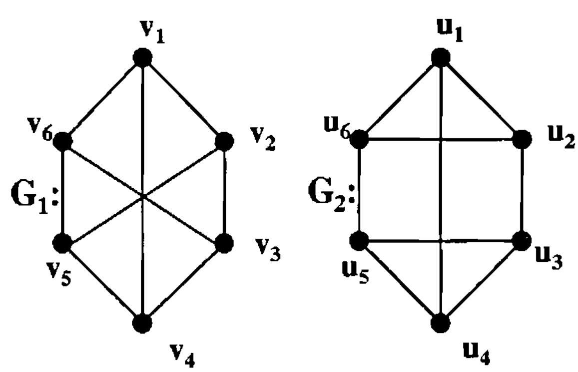


Figure 2.2: The graphs G_1 and G_2.

Now, replacing v_1 and u_1 in G_1 and G_2 by a triangle each we get two cubic graphs $\mathcal{H}_1$ and $\mathcal{H}_2$ on eight vertices containing one and two triangles respectively as shown in Figure 2.3. Since the number of triangles in a graph is the negative of half the coefficient of λ^{p-3} in its characteristic polynomial [24], $\mathcal{H}_1$ and $\mathcal{H}_2$ are non-cospectral.

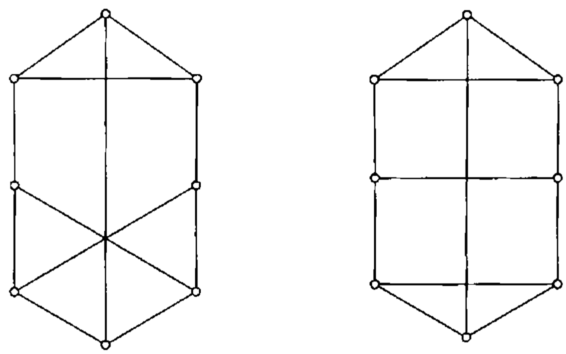


Figure 2.3: The graphs $\mathcal{H}_1$ and $\mathcal{H}_2$

Replacing any vertex in the newly formed triangle in $\mathcal{H}_1$ and $\mathcal{H}_2$ by a triangle we get two cubic graphs on ten vertices which are non-cospectral. Repeating this process $(t-3)$ times, we get two cubic graphs on $2t$ vertices containing one and two triangles respectively. Hence they are non-cospectral. □

Theorem 2.8. *For every $p = 24t + 1$, $t \geq 3$, there exists a pair of equienergetic self-complementary graphs.*

Proof. Let G_1 and G_2 be the two non-cospectral cubic graphs on $2t$ vertices given by Lemma 2.2. Let F_1 and F_2 respectively denote their second iterated line graphs. Then, F_1 and F_2 have $6t$ vertices each and $6-$regular with $\mathcal{E}(F_1) = \mathcal{E}(F_2) = 12t$ and $\mathcal{E}(\overline{F_1}) = \mathcal{E}(\overline{F_2}) = 3(6t-4) - 2$ by Lemma 1.15. Let $\mathcal{F}_1$ and $\mathcal{F}_2$ be the self-complementary graphs obtained from F_1 and F_2 by Construction 4. Then, $\mathcal{F}_1$ and $\mathcal{F}_2$ are on $p = 24t + 1$ vertices and by Corollary 2.2, $\mathcal{E}(\mathcal{F}_1) = \mathcal{E}(\mathcal{F}_2) =$

$2(24t-13)+\sqrt{169+144t^2}+T$ where T is the sum of the absolute values of the roots of the cubic $x^3-(12t-1)x^2-6(6t^2-10t+7)x+12t(12t-7)=0$. □

Equienergetic line graphs of self-complementary graphs

We shall now construct a pair of non-regular equienergetic graphs on $p(4p-1)$ vertices, $p \geq 4$ which are line graphs of self-complementary graphs.

Theorem 2.9. *Let G be an $r-$regular connected graph with $spec(G) = \{r, \lambda_2, ..., \lambda_p\}$, $p \geq 3$ and H_1 be the self-complementary graph obtained from G by Construction 1. Then, $\mathcal{E}(L(H_1)) = 4p(4p-5)$.*

Proof. Let A be an adjacency matrix of G. Then, adjacency matrix $\overline{A}$ of $\overline{G}$ is given by $\overline{A} = J - I - A$ where J is the all one matrix. By definition of H_1, its adjacency matrix and degree matrix can be written as

$$A(H_1) = \begin{bmatrix} A & J & 0 & 0 \\ J & \overline{A} & J & 0 \\ 0 & J & \overline{A} & J \\ 0 & 0 & J & A \end{bmatrix}$$

and

$$\hat{D}(H_1) = \begin{bmatrix} (p+r)\,I & 0 & 0 & 0 \\ 0 & (3p-r-1)\,I & 0 & 0 \\ 0 & 0 & (3p-r-1)\,I & 0 \\ 0 & 0 & 0 & (p+r)\,I \end{bmatrix}$$

Now, H_1 has $4p$ vertices and $p(4p-1)$ edges. By Lemma 1.8 the characteristic polynomial of $L(H_1)$ is given by $P_{L(H_1)}(\lambda-2) = \lambda^{\frac{p(3p-5)}{2}} \left|\lambda I - A(H_1) - \hat{D}(H_1)\right|$.

Now, $\left|\lambda I - A(H_1) - \hat{D}(H_1)\right|$

$$= \prod_{i=1}^{p} \left\{ \begin{array}{l} J^2 \left[\lambda - (p+r) - \lambda_i\right]^2 \\ - \left[J^2 - (\lambda - (p+r) - \lambda_i)\,(\lambda - (3p-r-2) - J + \lambda_i)\right]^2 \end{array} \right\}$$

by Lemmas 1.1 and 1.6 . So using Lemmas 1.7 and 1.8,

$$spec(L(H_1)) = \left(\begin{array}{ccc} 3\,(p-1) \pm \alpha & 2p-3 \pm \beta & 3p-4-(\lambda_i+r) \\ 1 & 1 & 1 \\ p-2+(\lambda_i+r) & -2 & \\ 1 & p(4p-5) & \end{array} \right), i = 2 \text{ to } p.$$

where $\alpha = \sqrt{(2p-2r-1)^2 + p^2}$ and $\beta = \sqrt{(p-2r-1)^2 + p^2}$.

Now, the two roots $3(p-1) \pm \alpha$ and $2p-3 \pm \beta$ are positive for $p \geq 3$. For $r \leq p-1$ the eigenvalues $3p-4-(\lambda_i+r)$ and $p-2+(\lambda_i+r)$ are positive as $\lambda_i + r \geq 0$, $i = 2, \ldots, p$. Thus, the only negative eigenvalue of $L(F)$ is -2 with multiplicity $p(4p-5)$. Thus, $\mathcal{E}[L(F)] = 4p(4p-5)$. □

Corollary 2.3. *Let G_1 and G_2 be any two regular connected graphs on p vertices, $p \geq 4$ and F_1, F_2 be the non-regular self-complementary graphs obtained from them by Construction 1. Then, $\mathcal{E}[L(F_1)] = \mathcal{E}[L(F_2)] = 4p(4p-5)$.*

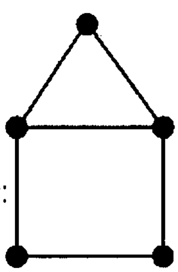
2.3 Equienergetic graphs from some graph operations

In this section we first consider some graphs whose spectrum is contained in $[-2k, 2k]$ for some k and then, use it to construct non-regular equienergetic graphs.

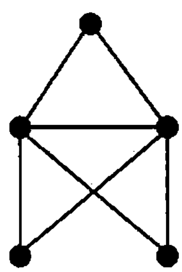
Examples:

1. G and H are two graphs on 5 vertices whose spectrum is contained in [-4,4].

G:



H:



$spec(G) = \{-2, -1.1701, 0, 0.6889, 2.4812\}$ $spec(H) = \{-2, -1, 0, 0, 3\}$

2. Let G be any $2k$ regular graph. Then, the spectrum of its vertex deleted subgraphs lies in $[-2k, 2k]$. This follows as a consequence of the interlacing theorem [34].

Theorem 2.10. *Let G be an $r-$ regular graph on p vertices with $r \geqslant 2(k+1)$. Then, for any graph F on n vertices whose spectrum is contained in $[-2k, 2k]$, $\mathcal{E}\left[\left\{L^2(G)\right\}^k \times F\right] = \frac{nk}{2^{k-2}}\left[pr(r-2)\right]^k$.*

Proof. By Lemma 1.14 and 1.15 the only negative eigenvalue of $\{L^2(G)\}^k$ is $-2k$ with multiplicity $\left[\frac{pr(r-2)}{2}\right]^k$ for $r \geq k+2$.
Let F be a graph whose spectrum is contained in $[-2k, 2k]$. Then, by Lemma 1.14, for $r \geqslant 2(k+1)$, the negative eigenvalues of $\left[\left\{L^2(G)\right\}^k \times F\right]$ are $-2k+\mu_i$, each with multiplicity $\left[\frac{pr(r-2)}{2}\right]^k$ where $\mu_i, i = 1$ to n are the eigenvalues of F. Thus, we get

$$\begin{aligned}\mathcal{E}\left[\left\{L^2(G)\right\}^k \times F\right] &= 2 \times \left[\frac{pr(r-2)}{2}\right]^k \sum_{i=1}^{n} |-2k+\mu_i| \\ &= \frac{nk}{2^{k-2}}\left[pr(r-2)\right]^k\end{aligned}$$

□

Corollary 2.4. *For any $r-$ regular graph G on p vertices, $r \geq 4$, $L^2(G) \times C_n$ and $L^2(G) \times P_n$ are equienergetic with energy $2pnr(r-2)$.*

Proof. Proof follows from the fact that the spectra of C_n and P_n lies in $[-2, 2]$. □

Corollary 2.5. *For any $r-$ regular graph G on p vertices, $r \geq 4$, $L^t(G) \times C_n$ and $L^t(G) \times P_n$ are equienergetic for $t \geq 3$.*

Proof. Since $L^t(G) = L^2(L^{t-2}(G))$, the claim follows from Corollary 2.4. □

Corollary 2.6. *Let F_1 and F_2 be non-isomorphic, non-regular graphs on n vertices whose spectrum is contained in $[-2k, 2k]$. Then, $\{L^2(G)\}^k \times F_1$ and $\{L^2(G)\}^k \times F_2$ are non-regular and equienergetic with energy $\frac{nk}{2^{k-2}}\left[pr(r-2)\right]^k$.*

Theorem 2.11. *Let m and k be positive integers with $m \geq 2k$. Then, for any graph G on p vertices whose spectrum is contained in $[-k, k]$,*
$\mathcal{E}\left[\{K_m\}^k \times G\right] = 2pk(m-1)^k$.

Proof. From Lemma 1.14 and 1.11 it follows that the $spec(\{K_m\}^k)$ is

$$\begin{pmatrix} km-k & (k-1)m-k & (k-2)m-k & & m-k & -k \\ 1 & kC_1(m-1) & kC_2(m-1)^2 & \ldots. & kC_1(m-1)^k & (m-1)^k \end{pmatrix}.$$

Since the spectrum of G is contained in $[-k, k]$, $\mu_i + k \geq 0$ for every $\mu_i \in spec(G)$. If $m \geq 2k$, then, by Lemma 1.14 the negative eigenvalues of $\{K_m\}^k \times G$ are $-k + \mu_i$, i =1 to p each with multiplicity $(m-1)^k$. Thus,

$$\begin{aligned} \mathcal{E}\left[\{K_m\}^k \times G\right] &= 2 \times (m-1)^k \times \sum_{i=1}^{p} |-k + \mu_i| \\ &= 2pk(m-1)^k \end{aligned}$$

□

Corollary 2.7. $\mathcal{E}(\{K_m\}^2 \times C_n) = \mathcal{E}(\{K_m\}^2 \times P_n) = 4n(m-1)^2$.

Corollary 2.8. *Let F_1 and F_2 be non-isomorphic, non-regular graphs on p vertices whose spectrum is contained in $[-k, k]$. Then, for every $m \geq 2k$, $\{K_m\}^k \times F_1$ and $\{K_m\}^k \times F_2$ are non-regular equienergetic with energy $2pk(m-1)^k$.*

Equienergetic non-regular line graphs

In [77] the construction of equienergetic regular line graphs is described. In this section we prove the existence of equienergetic non-regular line graphs.

Theorem 2.12. *Let G be an $r-$regular graph with $spec(G) = \{r, \lambda_2, ..., \lambda_p\}$, $p \geq 4$. Then, $\mathcal{E}(L[G\nabla\overline{G}]) = 2p(3p-5)$.*

Proof. Let A be an adjacency matrix of G. Then, by Lemma 1.3 $\overline{A} = J - I - A$ where J is the all one matrix.

Let $F = G\nabla\overline{G}$. Then, the adjacency matrix $A(F)$ and degree matrix $\hat{D}(F)$ of F can be written as

$$A(F) = \begin{bmatrix} A & J_p \\ J_p & \overline{A} \end{bmatrix} \text{ and } \hat{D}(F) = \begin{bmatrix} (p+r)\,I & 0_p \\ 0_p & (2p-r-1)\,I \end{bmatrix}.$$

Now, F has $2p$ vertices and $\frac{p(3p-1)}{2}$ edges. By Lemma 1.8 the characteristic polynomial of $L(F)$ is given by $P_{L(F)}\,(\lambda-2) = \lambda^{\frac{p(3p-5)}{2}}\left|\lambda I - A(F) - \hat{D}(F)\right|$.

Now,

$$\begin{aligned} &\left|\lambda I - A(F) - \hat{D}(F)\right| \\ &= \begin{vmatrix} \lambda I - ((p+r)\,I + A) & -J_p \\ -J_p & \lambda I - ((2p-r-2)\,I + J - A) \end{vmatrix} \\ &= \prod_{i=1}^{p} \left[\lambda - (p+r+\lambda_i)\right]\left[\lambda - (2p-r-2+J-\lambda_i)\right] - pJ \end{aligned}$$

So using Lemmas 1.6 and 1.7,

$$spec(L(F)) = \begin{pmatrix} 2p-3\pm\alpha & p-2+\lambda_i+r & 2p-4-(\lambda_i+r) & -2 \\ 1 & 1 & 1 & \frac{p(3p-5)}{2} \end{pmatrix}$$

$i = 2$ to p, where $\alpha = \sqrt{p^2 + (p-2r-1)^2}$.

Since G is $r-$regular, $\lambda_i + r < 2r \leq 2(p-2)$ if G is not complete and $\lambda_i + r = p - 2$ if G is complete. Also, the eigenvalues $2p - 3 \pm \alpha$ are always positive for $p \geq 4$. Thus, the only negative eigenvalue of $L(F)$ is -2 with multiplicity $\frac{p(3p-5)}{2}$. Hence $\mathcal{E}(L[G\nabla\overline{G}]) = 2 \times 2 \times \frac{p(3p-5)}{2} = 2p(3p-5)$. □

Corollary 2.9. *Let* $G_1 = C_p$ *and* $G_2 = K_p$. *Then,* $\mathcal{E}[L(C_p\nabla\overline{C_p})] = \mathcal{E}[L(K_p\nabla\overline{K_p})]$.

Chapter 3

Spectrum and energies of some graphs

In this chapter we obtain the following.

✠ The spectrum of some non-regular graphs and their complements.

✠ The energy of some non-regular graphs.

✠ The energy of $\overline{S}(C_p)$ and $\overline{C_p}$.

Some results of this chapter are included in
Energies of some non-regular graphs, J. Math. Chem., (to appear).

3.1 Spectrum of some non-regular graphs and their complements.

Let G be a graph. Consider the following seven operations on G and denote the resulting graphs by F_i,$i = 1, \ldots\ldots, 7$.

Operation 1. *Introduce a copy of $\overline{G}$ on $U = \{u_i\}$ corresponding to the vertices of G. Make u_i adjacent to v_i for each $i = 1, 2, \ldots, p$.*

Operation 2. *Introduce a set $U = \{u_i\}$ corresponding to the vertices of G. Make u_i adjacent to all the vertices in $\overline{N[v_i]}$ for each $i = 1, 2, \ldots, p$.*

Operation 3. *Introduce a set $U = \{u_i\}$ corresponding to the vertices of G. Make u_i adjacent to all the vertices in $\overline{N(v_i)}$ for each $i = 1, 2, \ldots, p$.*

Operation 4. *Attach a pendant vertex to each vertex of G. The resulting graph is called the pendant join graph of G. [Also referred to as G corona K_1 in [10].]*

Operation 5. *Take one copy of G on $U = \{u_i\}$ and a set $W = \{w_i\}$ of p isolated vertices corresponding to the vertices of G. Make u_i adjacent to v_i for each $i = 1, 2, \ldots, p$. Make w_i adjacent to both u_i and v_i for each $i = 1, 2, \ldots, p$.*

Operation 6. *Introduce a set $U = \{u_i\}$ corresponding to the vertices of G. Make u_i adjacent to all the vertices of G except v_i for each i.*

Operation 7. *Take a copy of $\overline{G}$ on $U = \{u_i\}$ corresponding to the vertices of G. make u_i adjacent to all the vertices in $\overline{N[v_i]}$ for each $i = 1, 2, \ldots, p$.*

Theorem 3.1. *Let G be a connected $r-$ regular with an adjacency matrix A and spectrum $\{r, \lambda_2, \lambda_3, \ldots\ldots\ldots, \lambda_p\}$. Let $F_i s$ be the graphs as described above. Then, the spectrum of F_i and its complement , $i = 1, 2, \ldots, 7$ are as follows.*

i	$spec(F_i)$	$spec(\overline{F_i})$
1	$\left\{\begin{matrix} \frac{(p-1) \pm \sqrt{(p-2r-1)^2+4}}{2}; \\ \frac{-1 \pm \sqrt{1+4(\lambda_i^2+\lambda_i+1)}}{2}; \lambda_i \neq r \end{matrix}\right\}$	$\left\{\begin{matrix} \frac{(p-1) \pm \alpha}{2}; \\ \frac{-1 \pm \sqrt{1+4\left[\lambda_i^2-\lambda_i+1\right]}}{2}; \lambda_i \neq r \end{matrix}\right\}$
2	$\left\{\begin{matrix} \frac{r \pm \sqrt{r^2+4(p-r-1)^2}}{2} \\ \frac{\lambda_i \pm \sqrt{5\lambda_i^2+8\lambda_i+4}}{2}; \lambda_i \neq r \end{matrix}\right\}$	$\left\{\begin{matrix} \frac{2(p-1)-r \pm \sqrt{r^2+4(r+1)^2}}{2} \\ \frac{-(2+\lambda_i) \pm \sqrt{5\lambda_i^2+8\lambda_i+4}}{2} \end{matrix}\right\}$
3	$\left\{\begin{matrix} \frac{r \pm \sqrt{r^2+4(p-r)^2}}{2} \\ \frac{1 \pm \sqrt{5}}{2}\lambda_i; \lambda_i \neq r \end{matrix}\right\}$	$\left\{\begin{matrix} \frac{2(p-1)-r(1 \pm \sqrt{5})}{2} \\ \frac{\left(1 \pm \sqrt{5}\right)\lambda_i - 2}{2}; \lambda_i \neq r \end{matrix}\right\}$
4	$\frac{\lambda_i \pm \sqrt{\lambda_i^2+4}}{2}$	$\left\{\begin{matrix} \frac{2(p-1)-r \pm \sqrt{r^2+4(p-1)^2}}{2} \\ \frac{-(\lambda_i+2) \pm \sqrt{\lambda_i^2+4}}{2}; \lambda_i \neq r \end{matrix}\right\}$
5	$\left.\begin{matrix} \lambda_i - 1 \\ \frac{\lambda_i+1 \pm \sqrt{(\lambda_i+1)^2+8}}{2} \end{matrix}\right\}$	$\left\{\begin{matrix} \frac{3(p-1)-r \pm \sqrt{[3(p-1)-r]^2+4r(p-1)}}{2} \\ -\lambda_i \\ \frac{-(3+\lambda_i) \pm \sqrt{(3+\lambda_i)^2-4\lambda_i}}{2}; \lambda_i \neq r \end{matrix}\right.$
6	$\left.\begin{matrix} \frac{r \pm \sqrt{r^2+4(p-1)^2}}{2} \\ \frac{\lambda_i \pm \sqrt{\lambda_i^2+4}}{2}; \lambda_i \neq r \end{matrix}\right\}$	$\left\{\begin{matrix} \frac{2(p-1)-r \pm \sqrt{r^2+4}}{2} \\ \frac{-(2+\lambda_i) \pm \sqrt{\lambda_i^2+4}}{2}; \lambda_i \neq r \end{matrix}\right.$
7	$\left.\begin{matrix} \frac{p-1 \pm \sqrt{(p-1)^2+4(p-r-1)(p-2r-1)}}{2} \\ \frac{-1 \pm \sqrt{1+4(1+\lambda_i)(1+2\lambda_i)}}{2} \end{matrix}\right\}$	$\left.\begin{matrix} \frac{p-2r-1 \pm \sqrt{(p-2r-1)^2-4r(p-r-1)+4(r+1)^2}}{2} \\ \frac{-1 \pm \sqrt{1+4(1+\lambda_i)(1+2\lambda_i)}}{2}; \lambda_i \neq r \end{matrix}\right\}$

where $\alpha = \sqrt{(p-1)^2 + 4\left[(p-1)^2 - (p-r-1)r\right]}$.

Proof. The Table 2 gives the adjacency matrices of the graphs F_i and its complement under each of the Operation i for $i = 1, \ldots .7$.

Table 2

i	$A(F_i)$	$A(\overline{F_i})$
1	$\begin{bmatrix} A & I \\ I & \overline{A} \end{bmatrix}$	$\begin{bmatrix} \overline{A} & J-I \\ J-I & A \end{bmatrix}$
2	$\begin{bmatrix} A & \overline{A} \\ \overline{A} & 0_p \end{bmatrix}$	$\begin{bmatrix} \overline{A} & A+I \\ A+I & J-I \end{bmatrix}$
3	$\begin{bmatrix} A & \overline{A}+I \\ \overline{A}+I & 0_p \end{bmatrix}$	$\begin{bmatrix} \overline{A} & A \\ A & J-I \end{bmatrix}$
4	$\begin{bmatrix} A & I \\ I & 0 \end{bmatrix}$	$\begin{bmatrix} \overline{A} & J-I \\ J-I & J-I \end{bmatrix}$
5	$\begin{bmatrix} A & I & I \\ I & A & I \\ I & I & 0 \end{bmatrix}$	$\begin{bmatrix} \overline{A} & J-I & J-I \\ J-I & \overline{A} & J-I \\ J-I & J-I & J-I \end{bmatrix}$
6	$\begin{bmatrix} A & J-I \\ J-I & 0 \end{bmatrix}$	$\begin{bmatrix} \overline{A} & I \\ I & J-I \end{bmatrix}$
7	$\begin{bmatrix} A & \overline{A} \\ \overline{A} & \overline{A} \end{bmatrix}$	$\begin{bmatrix} \overline{A} & A+I \\ A+I & A \end{bmatrix}$

Now, the theorem follows from Table 3 which gives the characteristic polynomials of F_i and $\overline{F_i}$ for $i = 1, 2, ...7$.

Table 3

i	$P(F_i)$	$P(\overline{F_i})$
1	$\prod_{i=1}^{p} \{[\lambda + 1 + \lambda_i - J]\,[\lambda - \lambda_i] - 1\}$	$\prod_{i=1}^{p} \{[\lambda - (J - 1 - \lambda_i)]\,[\lambda - \lambda_i] - (J - I)^2\}$
2	$\prod_{i=1}^{p} [\lambda^2 - \lambda_i\lambda - (J - I - \lambda_i)^2]$	$\prod_{i=1}^{p} \left\{\begin{matrix} [\lambda - (J - I - \lambda_i)]\,[\lambda - (J - I)] \\ -(\lambda_i + 1)^2 \end{matrix}\right\}$
3	$\prod_{i=1}^{p} [\lambda^2 - \lambda_i\lambda - (J - \lambda_i)^2]$	$\prod_{i=1}^{p} \{[\lambda - (J - I - \lambda_i)]\,[\lambda - (J - I)] - \lambda_i^2\}$
4	$\prod_{i=1}^{p} [\lambda^2 - \lambda_i\lambda - 1]$	$\prod_{i=1}^{p} \left[\begin{matrix} \lambda^2 - \{2\,(J - I) - \lambda_i\}\,\lambda \\ -\lambda_i\,(J - I) \end{matrix}\right]$
5	$\prod_{i=1}^{p} \left\{\begin{matrix} [\lambda - (\lambda_i - 1)] \\ \times\,[\lambda^2 - (\lambda_i + 1)\,\lambda - 2] \end{matrix}\right\}$	$\prod_{i=}^{p} (\lambda + \lambda_i) \left[\begin{matrix} \lambda^2 - \{3\,(J - I) - \lambda_i\}\,\lambda \\ -\lambda_i\,(J - I) \end{matrix}\right]$
6	$\prod_{i=1}^{p} [\lambda\,(\lambda - \lambda_i) - (J - I)^2]$	$\prod_{i=}^{p} [\{\lambda - (J - I - \lambda_i)\}\,\{\lambda - J + I\} - 1]$
7	$\prod_{i=1}^{p} \left\{\begin{matrix} (\lambda - \lambda_i)\,(\lambda - J + I + \lambda_i) \\ -(J - I - \lambda_i)^2 \end{matrix}\right\}$	$\prod_{i=1}^{p} \left\{\begin{matrix} (\lambda - \lambda_i)\,(\lambda - J + I + \lambda_i) \\ -(1 + \lambda_i)^2 \end{matrix}\right\}$

where $J = Q(\lambda_i)$ as given by Lemma 1.7. □

3.2 Energies of some non-regular graphs

Let G be a graph. We shall now consider the following six operations on G, denote the resulting non-regular graphs by H_i,$i = 8, 9, \ldots, 13$ and obtain expressions for the energies of these graphs in terms of the energy of G.

Operation 8. *Let G_1 be the duplication graph of G (Definition 17). Introduce k isolated vertices and make each of them adjacent to all the vertices of G only.*

Operation 9. *Introduce two sets $U = \{u_i\}$ and $W = \{w_i\}$ corresponding to the* *vertices of G. Make u_i adjacent to all the vertices in $N(v_i)$ and w_i adjacent to all the vertices in $\overline{N(v_i)}$ for each $i = 1, 2, \ldots, p$.*

Operation 10. *Introduce two sets $U = \{u_i\}$, $i = 1, 2, \ldots, p$ and $W = \{w_j\}$,$j = 1, 2, \ldots, k$. Make u_i adjacent to all the vertices in $\overline{N(v_i)}$ for each i and make every vertex of W adjacent to all the vertices of G.*

Operation 11. *Introduce two sets $U = \{u_i\}$ and $W = \{w_i\}$ corresponding to the vertices of G. Make u_i and w_i adjacent to all the vertices in $\overline{N(v_i)}$ for each $i = 1, 2, \ldots, p$.*

Operation 12. *Introduce two sets $U = \{u_i\}$ and $W = \{w_i\}$ corresponding to the vertices of G. Make u_i adjacent to all the vertices in $N(v_i)$ and w_i adjacent to all the vertices in $\overline{N(v_i)}$ for each $i = 1, 2, \ldots, p$. Then, delete the edges of G only.*

Operation 13. *Introduce two sets $U = \{u_i\}$, $i = 1, 2, \ldots, p$ and $W = \{w_j\}$,$j = 1, 2, \ldots, k$. Make u_i adjacent to all the vertices in $\overline{N(v_i)}$ for each i and make every vertex of W adjacent to all the vertices of G. Then, delete the edges of G only.*

Theorem 3.2. *Let G be a connected $r-$ regular graph with an adjacency matrix A and spectrum $\{r, \lambda_2, \lambda_3, \ldots\ldots\ldots, \lambda_p\}$. Let H_i, $i = 8, 9, \ldots, 13$ be the non-regular graphs described as above. Then,*

$$\mathcal{E}(H_8) = 2\left[\mathcal{E}(G) - r + \sqrt{r^2 + pk}\right]$$
$$\mathcal{E}(H_9) = 3\left(\mathcal{E}(G) - r\right) + \sqrt{r^2 + 4\left\{(p-r)^2 + r^2\right\}}$$
$$\mathcal{E}(H_{10}) = \sqrt{5}\left[\mathcal{E}(G) - r\right] + \sqrt{r^2 + 4\left(pk + \{p-r\}^2\right)}$$
$$\mathcal{E}(H_{11}) = 3\left[\mathcal{E}(G) - r\right] + \sqrt{r^2 + 8\left(p-r\right)^2}$$
$$\mathcal{E}(H_{12}) = 2\left\{\sqrt{2}\left(\mathcal{E}(G) - r\right) + \sqrt{r^2 + (p-r)^2}\right\}$$
$$\mathcal{E}(H_{13}) = 2\left[\mathcal{E}(G) - r + \sqrt{(p-r)^2 + pk}\right]$$

Proof. For each of the operations, using Lemmas 1.1, 1.6 and 1.7, the characteristic polynomial and the eigenvalues are given in Table 1.

Table 1

i	$A(H_i)$	$P(H_i)$	$spec(H_i)$
8	$\begin{bmatrix} 0_p & A & J_{p\times k} \\ A & 0_p & 0_{p\times k} \\ J_{k\times p} & 0_{k\times p} & 0_k \end{bmatrix}$	$\lambda^k \prod_{i=1}^{p} [\lambda^2 - kJ - \lambda_i^2]$	$\lambda = 0$; k times $= \pm\,\alpha_1$ $= \pm\lambda_i;\ \lambda_i \neq r$
9	$\begin{bmatrix} A & A & \overline{A}+I \\ A & 0_p & 0_p \\ \overline{A}+I & 0_p & 0_p \end{bmatrix}$	$\lambda^p \prod_{i=1}^{p} \begin{bmatrix} \lambda(\lambda-\lambda_i) \\ -(J-\lambda_i)^2 - \lambda_i^2 \end{bmatrix}$	$\lambda = 0$; p times $= \dfrac{r \pm \alpha_2}{2}$ $= 2\lambda_i, -\lambda_i;\ \lambda_i \neq r$
10	$\begin{bmatrix} A & \overline{A}+I & J_{p\times k} \\ \overline{A}+I & 0_p & 0_{p\times k} \\ J_{k\times p} & 0_{k\times p} & 0_k \end{bmatrix}$	$\lambda^k \prod_{i=1}^{p} \begin{Bmatrix} [\lambda(\lambda-\lambda_i) - kJ] \\ -[J-\lambda_i]^2 \end{Bmatrix}$	$\lambda = 0$; k times $= \dfrac{r \pm \alpha_3}{2}$ $= \dfrac{1 \pm \sqrt{5}}{2}\lambda_i; \lambda_i \neq r$
11	$\begin{bmatrix} A & \overline{A}+I & \overline{A}+I \\ \overline{A}+I & 0_p & 0_p \\ \overline{A}+I & 0_p & 0_p \end{bmatrix}$	$\lambda^p \prod_{i=1}^{p} \begin{bmatrix} \lambda(\lambda-\lambda_i) \\ -2(J-\lambda_i)^2 \end{bmatrix}$	$\lambda = 0$; p times $= \dfrac{r \pm \alpha_4}{2}$ $= 2\lambda_i, -\lambda_i\ ; \lambda_i \neq r$
12	$\begin{bmatrix} 0 & A & \overline{A}+I \\ A & 0 & 0 \\ \overline{A}+I & 0 & 0 \end{bmatrix}$	$\lambda^p \prod_{i=1}^{p} \begin{bmatrix} \lambda^2 - (J-\lambda_i)^2 \\ -\lambda_i^2 \end{bmatrix}$	$\lambda = 0$; p times $= \pm\alpha_5$ $= \pm\sqrt{2}\lambda_i\ ; \lambda_i \neq r$
13	$\begin{bmatrix} 0 & \overline{A}+I & J_{p\times k} \\ \overline{A}+I & 0 & 0 \\ J_{k\times p} & 0 & 0 \end{bmatrix}$	$\lambda^k \prod_{i=1}^{p} \begin{bmatrix} \lambda^2 - kJ \\ -(J-\lambda_i)^2 \end{bmatrix}$	$\lambda = 0$; k times $= \pm\alpha_6$ $= \pm\lambda_i\ ; \lambda_i \neq r$

By Lemma 1.7, $J = Q(\lambda_i)$. Also, in column 4, $\alpha_1 = \sqrt{r^2 + pk}$,
$\alpha_2 = \sqrt{r^2 + 4\left[(p-r)^2 + r^2\right]}$, $\alpha_3 = \sqrt{r^2 + 4\left[pk + (p-r)^2\right]}$, $\alpha_4 = \sqrt{r^2 + 8(p-r)^2}$,
$\alpha_5 = \sqrt{r^2 + (p-r)^2}$ and $\alpha_6 = \sqrt{pk + (p-r)^2}$. Hence, the theorem. □

3.3 Partial complement of the subdivision graph

In this section we obtain the spectrum of the partial complement of the subdivision graph $\overline{S}(G)$ of a regular graph G and energy of $\overline{S}(C_p)$.

Lemma 3.1. *Let G be an $r-$ regular graph with an adjacency matrix A and incidence matrix R. Then, $\overline{R} = J_{p\times q} - R$, $\overline{R}^T = J_{q\times p} - R^T$ and $R\overline{R}^T = (q-2r)\,J + (A+r)$.*

Proof. By Definition 32, $\overline{R} = J_{p\times q} - R$. Therefore

$$\begin{aligned}
\overline{R}\,\overline{R}^T &= (J_{p\times q} - R)\left(J_{q\times p} - R^T\right)\\
&= qJ - rJ - rJ + A + rI\\
&= (q-2r)\,J + (A+r)I, \text{ by Lemma 1.4}
\end{aligned}$$

Hence the lemma. □

Lemma 3.2. *Let G be a connected $r-$regular (p,q) graph. Then, $\overline{S}(G)$ is regular if and only if G is a cycle.*

Proof. From Definition 33, we have the degree of vertices in $\overline{S}(G)$ corresponding to the edges of G is $p-2$ each and of those corresponding to the vertices of G is $q-r$ each. Since G is $r-$ regular, $q = \frac{pr}{2}$ and hence $q - r = p - 2$ if and only if $r = 2$. Thus, $\overline{S}(G)$ is regular if and only if G is a cycle. □

Theorem 3.3. *Let G be a connected $r-$ regular (p,q) graph. Then,*

$$spec(\overline{S}(G)) = \begin{pmatrix} \pm\sqrt{p\,(q-2r)+2r} & \pm\sqrt{\lambda_i + r} & 0 \\ 1 & 1 & q-p \end{pmatrix}, i = 2 \text{ to } p.$$

Proof. The adjacency matrix of $\overline{S}(G)$ can be written as $\begin{bmatrix} 0 & \overline{R} \\ \overline{R}^T & 0 \end{bmatrix}$. Then, the theorem follows from Lemmas 1.1 and 3.1. □

Theorem 3.4.

$$\mathcal{E}\left(\overline{S}\left(C_p\right)\right) = \begin{cases} 2\left(p-4+2\cot\frac{\pi}{2p}\right), p \text{ even} \\ \\ 2\left(p-4+2cosec\,\frac{\pi}{2p}\right), p \text{ odd} \end{cases}$$

Proof. By Lemma 1.11 and Theorem 3.3 we have

$$spec\left(\overline{S}\left(C_p\right)\right) = \begin{pmatrix} p-2 & -(p-2) & \pm 2\cos\frac{\pi j}{p} \\ 1 & 1 & 1 \end{pmatrix}, j = 1 \text{ to } p-1.$$

We shall consider the following two cases.

Case 1. $p \equiv 0(mod\ 2)$.

The cosine numbers $2cos\frac{\pi j}{p}$ are positive only for $\frac{\pi}{p}j \leq \frac{\pi}{2}$. Then, the positive cosine numbers are $2\cos\frac{\pi}{p}, 2\cos\left(\frac{\pi}{p}\times 2\right), \ldots\ldots\ldots\ldots, 2\cos\left(\frac{\pi}{p}\times\frac{p}{2}\right)$.

Let $C = 2\cos\frac{\pi}{p} + 2\cos\left(\frac{\pi}{p}\times 2\right) + \ldots\ldots\ldots + 2\cos\left(\frac{\pi}{p}\times\frac{p}{2}\right)$ and
$S = 2\sin\frac{\pi}{p} + 2\sin\left(\frac{\pi}{p}\times 2\right) + \ldots\ldots\ldots + 2\sin\left(\frac{\pi}{p}\times\frac{p}{2}\right)$

so that

$$\begin{aligned} C + iS &= 2\gamma + 2\gamma^2 + ... + 2\gamma^{\frac{p}{2}} \\ &= 2\gamma \frac{(1 - \gamma^{\frac{p}{2}})}{1 - \gamma} \end{aligned}$$

where $\gamma = \cos\frac{\pi}{p} + i \sin\frac{\pi}{p}$ and $i = \sqrt{-1}$.

Now, equating real parts, we get $C = \cot\frac{\pi}{2p} - 1$. Since the spectrum of $\left(\overline{S}\left(C_p\right)\right)$ is symmetric with respect to zero, the energy contribution from the cosine numbers is $2C$. Thus,

$$\begin{aligned} \mathcal{E}\left(\overline{S}\left(C_p\right)\right) &= 2 \times (p - 2 + 2C) \\ &= 2\left(p - 4 + 2\cot\frac{\pi}{2p}\right) \end{aligned}$$

Case 2. $p \equiv 1 (mod\ 2)$.

When p is odd, the cosine numbers $2cos\frac{\pi j}{p}$ are positive for $j \leq \frac{p-1}{2}$. Then, by a similar argument as in Case 1, we get $\mathcal{E}(\overline{S}(C_p)) = 2\left(p - 4 + 2\cos ec\frac{\pi}{2p}\right)$. $\square$

3.4 Energy of $\overline{C_p}$

In this section we derive an analytic expression for the energy of $\overline{C_p}$.

Theorem 3.5.

$$\mathcal{E}\left(\overline{C_p}\right) = \begin{cases} 2\left(\frac{2p-9}{3} + \sqrt{3}\cot\frac{\pi}{p}\right); p \equiv 0(mod\ 3) \\ \\ 2\left(\frac{2p-8}{3} + \frac{2\sin\frac{\pi}{3}\left(1-\frac{1}{p}\right)}{\sin\frac{\pi}{p}}\right); p \equiv 1(mod\ 3) \\ \\ 2\left(\frac{2p-10}{3} + \frac{2\sin\frac{\pi}{3}\left(1+\frac{1}{p}\right)}{\sin\frac{\pi}{p}}\right); p \equiv 2(mod\ 3) \\ \end{cases}$$

Proof. We have $spec(\overline{C_p}) = \begin{pmatrix} p-3 & -\left(1+2\cos\frac{2\pi j}{p}\right) \\ 1 & 1 \end{pmatrix}, j = 1\ to\ p-1$ by Lemmas 1.11 and 1.12.

We shall consider the following cases.

Case 1. $p \equiv 0(mod\ 3)$.

Then, $-\left(1+2\cos\frac{2\pi j}{p}\right) \geq 0$ if and only if $\frac{p}{3} \leq j \leq \frac{2p}{3}$.
Let $\sum\limits_{j=\frac{p}{3}}^{\frac{2p}{3}} \left(1+2\cos\frac{2\pi j}{p}\right) = \frac{p+3}{3} + \sum\limits_{j=\frac{p}{3}}^{\frac{2p}{3}} 2\cos\frac{2\pi j}{p} = \frac{p+3}{3} + C$ and
$S = \sum\limits_{j=\frac{p}{3}}^{\frac{2p}{3}} 2\sin\frac{2\pi j}{p}$, so that $C + iS = \sum\limits_{j=\frac{p}{3}}^{\frac{2p}{3}} \gamma^j$ where $\gamma = \cos\frac{2\pi}{p} + i\sin\frac{2\pi}{p}$.
Equating real parts, we get $C = -(1+\sqrt{3}\ cot\frac{\pi}{p})$.

The total sum of positive eigenvalues

$$\begin{aligned}
&= p - 3 + \sqrt{3}\cot\frac{\pi}{p} + 1 - \left(\frac{p+3}{3}\right) \\
&= \frac{2p-9}{3} + \sqrt{3}\cot\frac{\pi}{p}.
\end{aligned}$$

Thus, $\mathcal{E}(\overline{C_p}) = 2 \times [\frac{2p-9}{3} + \sqrt{3}\cot\frac{\pi}{p}]$.

The other two cases $p \equiv 1(mod\ 3)$ and $p \equiv 2(mod\ 3)$ can be proved similarly . $\square$

Chapter 4

Reciprocal graphs

In this chapter we obtain

- Some new classes of reciprocal graphs.
- An upperbound for the energy of reciprocal graphs.
- Pair of equienergetic reciprocal graphs for every $p \equiv 0(mod\ 12)$, $p \geq 36$ and $p \equiv 0(mod\ 16)$, $p \geq 48$.
- The Wiener indices of some reciprocal graphs.

4.1 New reciprocal graphs

We consider the following operations on G.

Operation 1. *Operation 4 as in Chapter 3.*

Operation 2. *The splitting graph of G(Definition 16).*

Operation 3. *In addition to G introduce two sets of p isolated vertices $U = \{u_i\}$ and $W = \{w_i\}$ corresponding to $V = \{v_i\}$, $i = 1$ to p. Make u_i and w_i adjacent to all the vertices in $N(v_i)$ and then, make w_i adjacent to all the vertices in U corresponding to the vertices of $N(v_i)$ in G for each $i = 1$ to p. The resulting graph is called the* ***double splitting graph*** *of G.*

Operation 4. *In addition to G introduce two more copies of G on $U = \{u_i\}$ and $W = \{w_i\}$ corresponding to $V = \{v_i\}$, $i = 1$ to p. Make u_i adjacent to all the vertices in $N(v_i)$ and then, make w_i adjacent to u_i for each $i = 1$ to p. The resulting graph is called the* ***composition graph*** *of G.*

Operation 5. *In addition to G introduce two more copies of G on $U = \{u_i\}$ and $W = \{w_i\}$ corresponding to $V = \{v_i\}$, $i = 1$ to p. Make w_i adjacent to all the vertices in $N(v_i)$ and the vertices in U corresponding to the vertices of $N(v_i)$ in G for each $i = 1$ to p.*

Lemma 4.1. *Let G be a graph on p vertices with $spec(G) = \{\lambda_1, \ldots, \lambda_p\}$ and H_i be the graph obtained from Operation i, $i = 1$ to 5. Then,*

$$spec(H_1) = \left\{ \frac{\lambda_i \pm \sqrt{\lambda_i^2 + 4}}{2} \right\}_{i=1}^{p}$$

$$spec(H_2) = \left\{ \left(\frac{1 \pm \sqrt{5}}{2} \right) \lambda_i \right\}_{i=1}^{p}$$

$$spec(H_3) = \left\{-\lambda_i, \left(1 \pm \sqrt{2}\right) \lambda_i\right\}_{i=1}^{p}$$
$$spec(H_4) = \left\{\lambda_i, \lambda_i \pm \sqrt{\lambda_i^2 + 1}\right\}_{i=1}^{p}$$
$$spec(H_5) = \left\{\lambda_i, \left(1 \pm \sqrt{2}\right) \lambda_i\right\}_{i=1}^{p}$$

Proof. The proof follows from the Table 1 which gives the adjacency matrix of $H_i s$ for $i = 2$ to 5 and its spectrum, obtained using Lemmas 1.1 and 1.13. The $spec(H_1)$ has been already mentioned in the proof of Theorem 3.1.

Table 1

Graph	$A(H_i)$	$spec(H_i)$
H_2	$\begin{bmatrix} A & A \\ A & 0 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \otimes A$	$\left\{\left(\frac{1\pm\sqrt{5}}{2}\right) \lambda_i\right\}_{i=1}^{p}$
H_3	$\begin{bmatrix} A & A & A \\ A & 0 & A \\ A & A & 0 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \otimes A$	$\{-\lambda_i, (1 \pm \sqrt{2}) \lambda_i\}_{i=1}^{p}$
H_4	$\begin{bmatrix} A & A & 0 \\ A & A & I \\ 0 & I & A \end{bmatrix}$	$\left\{\lambda_i,\ \lambda_i \pm \sqrt{\lambda_i^2 + 1}\right\}_{i=1}^{p}$
H_5	$\begin{bmatrix} A & 0 & A \\ 0 & A & A \\ A & A & A \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \otimes A$	$\{\lambda_i, (1 \pm \sqrt{2}) \lambda_i\}_{i=1}^{p}$

□

Note: $H_3 = H_5$, when G is bipartite.

Theorem 4.1. *The pendant join graph of a graph G is reciprocal if and only if G is bipartite.*

Proof. Let G be a bipartite graph and H, its pendant join graph. Then, corresponding to a non-zero eigenvalue λ of G, $-\lambda$ is also an eigenvalue of G [24].
By Lemma 4.1, $spec(H) = \{\frac{\lambda \pm \sqrt{\lambda^2+4}}{2},\ \lambda \in\ spec(G)\}$. Let $\alpha = \frac{\lambda+\sqrt{\lambda^2+4}}{2}$ be an eigenvalue of H. Then,

$$
\begin{aligned}
\frac{1}{\alpha} &= \frac{2}{\lambda+\sqrt{\lambda^2+4}} \\
&= \frac{2\left(\lambda-\sqrt{\lambda^2+4}\right)}{\left(\lambda+\sqrt{\lambda^2+4}\right)\left(\lambda-\sqrt{\lambda^2+4}\right)} \\
&= \frac{2\left(\lambda-\sqrt{\lambda^2+4}\right)}{-4} \\
&= \frac{(-\lambda)+\sqrt{(-\lambda)^2+4}}{2}
\end{aligned}
$$

is an eigenvalue of H as $-\lambda$ is an eigenvalue of G. Similarly for $\alpha = \frac{\lambda-\sqrt{\lambda^2+4}}{2}$ also. The eigenvalues of H corresponding to the zero eigenvalues of G if any, are 1 and -1 which are self reciprocal. Therefore H is a reciprocal graph.
The converse can be proved by retracing the argument. □

Note: This theorem enlarges the classes of reciprocal graphs mentioned in [85]. The claim in [85] that the pendant join graph of C_n is reciprocal for every n is not correct as C_n is not bipartite for odd n.

Theorem 4.2. *The splitting graph of G is reciprocal if and only if G is partially reciprocal.*

Proof. Let G be partially reciprocal and H be its splitting graph. Let $\alpha \in spec(H)$. Then, by Lemma 4.1, $\alpha = \left(\frac{1\pm\sqrt{5}}{2}\right)\lambda$, $\lambda \in spec(G)$. Without loss of generality, take $\alpha = \left(\frac{1+\sqrt{5}}{2}\right)\lambda$. Then, $\frac{1}{\alpha} = \left(\frac{1-\sqrt{5}}{2}\right)\frac{-1}{\lambda}$. Thus, $\frac{1}{\alpha} \in spec(H)$ as G is partially reciprocal and hence H is reciprocal.
Conversely assume that H is reciprocal. Then, by the structure of $spec(H)$ as given by Lemma 4.1, G is partially reciprocal. □

Theorem 4.3. *Let G be a reciprocal graph. Then, the double splitting graph and the composition graph of G are reciprocal if and only if G is bipartite.*

Proof. Let G be a bipartite reciprocal graph. Then, $\lambda \in spec(G) \Rightarrow -\lambda, \frac{1}{\lambda}, \frac{-1}{\lambda} \in spec(G)$. Let H and H' respectively denote the double splitting graph and composition graph of G. Then, from Lemma 4.1 and Table 2 it follows that H and H' are reciprocal.

Table 2

$spec(H)$	$\frac{1}{spec(H)}$
$\{-\lambda, (1\pm\sqrt{2})\,\lambda\}$	$\{-\frac{1}{\lambda}, (1\pm\sqrt{2})\,\frac{-1}{\lambda}\}$
$spec(H')$	$\frac{1}{spec(H')}$
$\left\{\lambda, \lambda \pm \sqrt{\lambda^2+1}\right\}$	$\left\{\frac{1}{\lambda}, -\lambda \pm \sqrt{(-\lambda)^2+1}\right\}$

The converse also follows. □

Illustration: The following graphs are reciprocal when $G = P_4$.

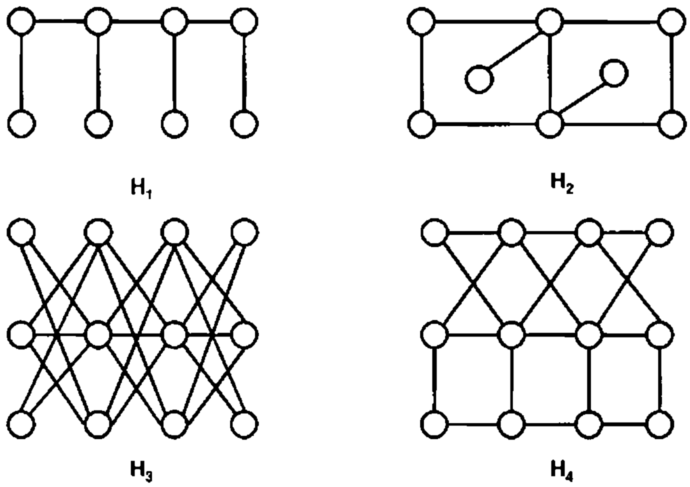


Figure 4.1:

4.2 An upperbound for the energy of reciprocal graphs

The following bounds on the energy of a graph are known.

1. [71] $\sqrt{2q + p(p-1)\,|\det A|^{\frac{2}{p}}} \leqslant E(G) \leqslant \sqrt{2pq}$
2. [62] $E(G) \leqslant \frac{2q}{p} + \sqrt{(p-1)\left(2q - 4\frac{q^2}{p^2}\right)}$
3. [63] $E(G) \leqslant \frac{4q}{p} + \sqrt{(p-2)\left(2q - 8\frac{q^2}{p^2}\right)}$, if G is bipartite.

In this section we derive a better upperbound for the energy of a reciprocal graph and prove that the bound is best possible.

Theorem 4.4. *Let G be a (p, q) reciprocal graph. Then, $\mathcal{E}(G) \leq \sqrt{\frac{p(2q+p)}{2}}$ and the bound is best possible for $G = tK_2$ and tP_4.*

Proof. Let G be a (p, q) reciprocal graph with $spec(G) = \{\lambda_1, \ldots, \lambda_p\}$.
Therefore $\sum_{i=1}^{p} |\lambda_i| = \sum_{i=1}^{p} \frac{1}{|\lambda_i|} = \mathcal{E}$ and $\sum_{i=1}^{p} \lambda_i^2 = \sum_{i=1}^{p} \frac{1}{\lambda_i^2} = 2q$.
Now, we have [92]the following inequality for real sequences a_i, b_i and c_i, $1 \leq i \leq n$

$$\sum_{i=1}^{n} a_i c_i \sum_{i=1}^{n} b_i c_i \leq \frac{1}{2} \left\{ \sum_{i=1}^{n} a_i b_i + \left(\sum_{i=1}^{n} a_i^2 \right)^{1/2} \left(\sum_{i=1}^{n} b_i^2 \right)^{1/2} \right\} \sum_{i=1}^{n} c_i^2$$

Taking $a_i = |\lambda_i|, b_i = \frac{1}{|\lambda_i|}$ and $c_i = 1 \ \forall i = 1, 2, \ldots, p$,
we have $[\mathcal{E}(G)]^2 \leq \frac{1}{2} [p + 2q] p$ and hence $\mathcal{E}(G) \leq \sqrt{\frac{p(2q+p)}{2}}$.
When $G = tK_2$, $p = 2t$, $q = t$, $\mathcal{E}(G) = 2t$ and when $G = tP_4$, $p = 4t$, $q = 3t$, $\mathcal{E}(G) = 2t\sqrt{5}$. □

4.3 Equienergetic reciprocal graphs

In this section we prove the existence of a pair of equienergetic reciprocal graphs on every $p = 12n$ and $p = 16n$, $n \geq 3$.

Theorem 4.5. *Let G be K_n, $n \geq 3$ and F_1 be the graph obtained by applying Operations 3, 1 and 2 on G and F_2, the graph obtained by applying Operations 5, 1 and 2 on G successively. Then, F_1 and F_2 are reciprocal and equienergetic on $12n$ vertices.*

Proof. Let $G = K_n$. We have $spec(K_n) = \begin{pmatrix} n-1 & -1 \\ 1 & n-1 \end{pmatrix}$.
Let G_3 be the graph obtained by applying Operation 3 on G.

Then, by Lemma 4.1,

$$spec(G_3) = \begin{pmatrix} -(n-1) & 1 & \left(1 \pm \sqrt{2}\right)(n-1) & -\left(1 \pm \sqrt{2}\right) \\ 1 & n-1 & 1 & n-1 \end{pmatrix}.$$

Now, let G_{31} be the graph obtained by applying Operation 1 on G_3. Then, by Lemma 4.1 $spec(G_{31})$ is

$$\begin{pmatrix} \frac{n-1\pm\sqrt{(n-1)^2+4}}{2} & \frac{-1\pm\sqrt{5}}{2} & \frac{\alpha\pm\sqrt{\alpha^2+4}}{2} \\ 1 & n-1 & 1 \\ & & \\ \frac{\beta\pm\sqrt{\beta^2+4}}{2} & \frac{(1+\sqrt{2})\pm\sqrt{\left\{(1+\sqrt{2})\right\}^2+4}}{2} & \frac{(1-\sqrt{2})\pm\sqrt{\left\{(1-\sqrt{2})\right\}^2+4}}{2} \\ 1 & n-1 & n-1 \end{pmatrix}$$

where $\alpha = \left(1 + \sqrt{2}\right)(n-1)$ and $\beta = \left(1 - \sqrt{2}\right)(n-1)$.

Then,

$$\begin{aligned} \mathcal{E}(G_{31}) &= \sqrt{(n-1)^2+4} + \sqrt{5}\,(n-1) + \sqrt{\left\{\left(1+\sqrt{2}\right)(n-1)\right\}^2+4} \\ &+\sqrt{\left\{\left(1-\sqrt{2}\right)(n-1)\right\}^2+4} + (n-1)\left[\sqrt{\left(1+\sqrt{2}\right)^2+4} + \sqrt{\left(1-\sqrt{2}\right)^2+4}\right] \\ &=\sqrt{(n-1)^2+4} + \sqrt{5}\,(n-1) + (n-1)\sqrt{14+2\sqrt{41}} \\ &+\sqrt{6\,(n-1)^2+8+2\sqrt{(n-1)^4+24\,(n-1)^2+16}} \end{aligned}$$

Now, let F_1 be the graph obtained by applying Operation 2 on G_{31}. Then, by Lemma 4.1, $\mathcal{E}(F_1) = \sqrt{5}\mathcal{E}(G_{31})$.

Let G_{51} be the graph obtained by applying Operations 5 and 1 on G successively and F_2 be that obtained by applying Operation 2 on G_{51}. Then, we have $\mathcal{E}(F_2) = \sqrt{5}\mathcal{E}(G_{51}) = \sqrt{5}\mathcal{E}(G_{31}) = \mathcal{E}(F_1)$. Also, by Theorem 4.2, F_1 and F_2 are reciprocal. Thus, the theorem follows. □

Lemma 4.2. *Let G be a non-bipartite graph on n vertices with $spec(G) = \{\lambda_1, \ldots, \lambda_n\}$ and an adjacency matrix A. Then, the spectra of graphs whose adjacency matrices are*

$$F' = \begin{bmatrix} A & A & A & A \\ A & A & 0 & A \\ A & 0 & A & A \\ A & A & A & 0 \end{bmatrix} \text{ and } H' = \begin{bmatrix} 0 & A & A & A \\ A & 0 & A & A \\ A & A & A & A \\ A & A & A & 0 \end{bmatrix} \text{ are}$$

$\left\{\lambda_i, -\lambda_i, \left(\frac{3\pm\sqrt{13}}{2}\right)\lambda_i\right\}_{i=1}^{n}$ *and* $\left\{-\lambda_i, -\lambda_i, \left(\frac{3\pm\sqrt{13}}{2}\right)\lambda_i\right\}_{i=1}^{n}$ *respectively .*

Theorem 4.6. *Let G be K_n, $n \geq 3$. Let T_1 and T_2 be the graphs obtained by applying Operations 1 and 2 successively on graphs associated with F' and H' respectively. Then, T_1 and T_2 are reciprocal and equienergetic on $16n$ vertices.*

Proof. Let the graph associated with F' be also denoted by F' and F_1', the graph obtained by applying Operation 1 on F'. Then, by a similar computation as in Theorem 4.5,

$$\begin{aligned}\mathcal{E}(F_1') = {} & 2\sqrt{(n-1)^2+4} + 2\sqrt{5}\,(n-1) + \sqrt{\left(\frac{11+3\sqrt{13}}{2}\right)(n-1)^2+4} \\ & + \sqrt{\left(\frac{11-3\sqrt{13}}{2}\right)(n-1)^2+4} \\ & + (n-1)\left[\sqrt{\left(\frac{11+3\sqrt{13}}{2}\right)+4} + \sqrt{\left(\frac{11-3\sqrt{13}}{2}\right)+4}\right]\end{aligned}$$

and $\mathcal{E}(T_1) = \sqrt{5}\mathcal{E}(F_1') = \sqrt{5}\mathcal{E}(H_1') = \mathcal{E}(T_2)$, by Lemma 4.1. Also, by Theorem 4.2, T_1 and T_2 are reciprocal. Hence the theorem. □

4.4 Wiener index of some reciprocal graphs

In this section we derive the Wiener indices of some classes of reciprocal graphs described in the earlier section. We shall denote by $\mathcal{D}(G) = \mathcal{D}$, the distance matrix of G and t_i, the sum of entries in the i^{th} row of $\mathcal{D}$. The following theorem generalizes the results in [70].

Theorem 4.7. *Let G be a graph with Wiener index $W(G)$. Let H be the pendant join graph of G. Then, $W(H) = 4W(G) + p(2p-1)$.*

Proof. We have, $W(G) = \frac{1}{2}\sum_{i=1}^{p} t_i$.
Let $V(G) = \{v_1, v_2, \ldots, v_p\}$ and $U = \{u_1, u_2, \ldots, u_p\}$ be the corresponding vertices used in the pendant join of G. Let $d_{ij} = d(v_i, v_j)$.
Then, the distance matrix of H is as follows.

$$\left[\begin{array}{ccc|ccc}
0 & d_{12} & d_{1p} & 1 & 1+d_{12} & 1+d_{1p} \\
 & & & & & \\
d_{p1} & .. \quad .. & 0 & 1+d_{p1} & .. \quad .. & 1 \\
\hline
1 & 1+d_{12} & 1+d_{1p} & 0 & 2+d_{12} \quad .. & 2+d_{1p} \\
 & & & & & \\
1+d_{p1} & & & 2+d_{p1} & & 0
\end{array}\right]$$

$$\begin{aligned}
\text{since } \; d(v_i, u_j) &= 1; \text{ if } i = j \\
&= 1 + d_{ij}; i \neq j \text{ and} \\
d(u_i, u_j) &= d(u_i, v_i) + d_{ij} + d(v_j, u_j) = 2 + d_{ij}
\end{aligned}$$

The row sum matrix of H is $\begin{bmatrix} 2t_1 + p \\ \\ \\ 2t_p + p \\ 2t_1 + 3p - 2 \\ \\ \\ 2t_p + 3p - 2 \end{bmatrix}$.

$$\text{Then, } W(H) = \frac{1}{2}\left[\sum_{i=1}^{p}(2t_i + p) + \sum_{i=1}^{p}(2t_i + 3p - 2)\right]$$

$$= 4W(G) + p(2p - 1). \text{ Hence the theorem.}$$

□

The proof techniques of the following theorems are on similar lines.

Theorem 4.8. *Let G be a triangle free (p, q) graph and H, its splitting graph. Then, $W(H) = 4W(G) + 2(p + q)$.*

Corollary 4.1. *Let G be a triangle free (p, q) graph and F, the splitting graph of the pendant join graph of G. Then, $W(F) = 2[8W(G) + 4p^2 + (p + q)]$.*

Theorem 4.9. *Let G be a triangle free (p, q) graph and H, its composition graph. Then, $W(H) = 9W(G) + 2p^2 + 4p$.*

Theorem 4.10. *Let G be a triangle free (p, q) graph and H, its double splitting graph. Then, $W(H) = 9W(G) + 6p + 4q$.*

Chapter 5

Integral graphs

In this chapter we obtain

- New integral graphs.
- Pair of equienergetic integral graphs on every $p \equiv 0 (mod\ 4)$ vertices.
- New integral split graphs.

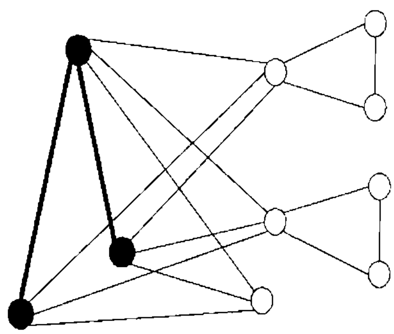
5.1 New integral graphs

Let G be a graph on p vertices and H be a graph rooted at v.

Operation 1. *Consider the graph obtained by identifying the roots in each of the k copies of H. The resulting graph is denoted by H_v^k.*

Some results of this chapter are included in
Some new integral graphs, Applicable Analysis and Discrete Mathematics,(to appear)

Operation 2. *Consider the graph obtained by joining each of the roots in k copies of H to all the vertices of G. This graph can be obtained by first forming the complete product $G\nabla\overline{K_k}$ and then, successively identifying the vertices in $\overline{K_k}$ one by one with v in the k copies of H. This is denoted by $k *_G H$. If only, t of the k vertices are identified, then, the resulting graph is denoted by F_k^t. Then, $F_k^0 = G\nabla\overline{K_k}$ and $F_k^k = k *_G H$.*



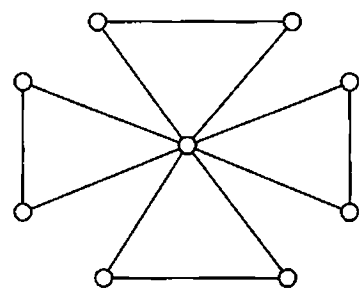


Figure 5.1: F_3^2; $G = K_{1,2}$; $H = K_3$ H_v^4 when $H = K_3$

Theorem 5.1. $P(H_v^k) = [P(H-v)]^{k-1}[kP(H) - (k-1)\lambda P(H-v)]$.

Proof. We shall prove the theorem by mathematical induction on k. The theorem is trivially true when $k = 1$. Assume that the result is true for $t < k$.

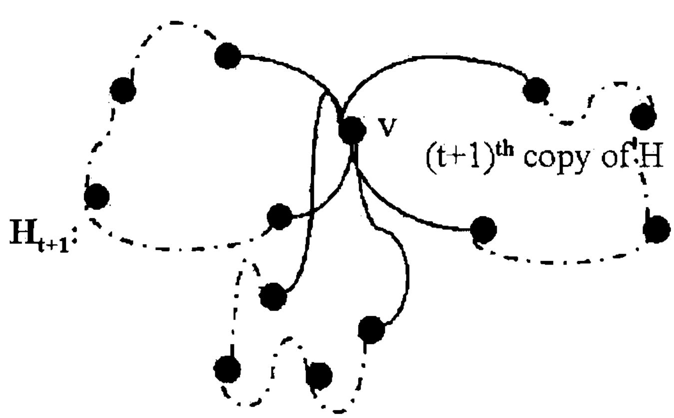


Figure 5.2:

Now,

$$\begin{aligned}
P\left(H_v^{t+1}\right) &= P(H)\left[P(H-v)\right]^t + P(H-v)\,P(H_t) - \lambda P(H-v)\left[P(H-v)\right]^t \\
&= P(H)\left[P(H-v)\right]^t \\
&\qquad + P(H-v) \times \left[\left(P(H-v)\right)^{t-1}\left\{tP(H) - (t-1)\lambda P(H-v)\right\}\right] \\
&= \left(P(H-v)\right)^t\left[(t+1)P(H) - t\lambda P(H-v)\right]
\end{aligned}$$

by the induction hypothesis and Lemma 1.10.

Hence the theorem is true for $t+1$ and by mathematical induction the theorem follows. □

Theorem 5.2. *Let G be an $r-$ regular graph on p vertices and H be rooted at v. Then, with the notations as described above*

$$P\left(F_k^t\right) = \frac{P(G)}{(\lambda - r)}\lambda^{k-(t+1)}\left[P(H)\right]^{t-1}\left[P(H)\left\{\lambda(\lambda-r) - p(k-t)\right\} - tp\lambda P(H-v)\right].$$

Proof. We shall prove the theorem by mathematical induction on t.

When $t = 0$, $F_k^0 = G\nabla\overline{K_k}$ and in this case $P\left(F_k^0\right) = \frac{P(G)}{(\lambda-r)}\lambda^{k-1}\left[\lambda(\lambda-r) - pk\right]$, which is true from Lemma 1.9.

Now, assume that the theorem is true when $t = s < k$. Now, by Lemma 1.10 and by the induction hypothesis

$$\begin{aligned}
P(F_k^{s+1}) &= P(F_k^s)P(H-v) + P(F_{k-1}^s)P(H) - \lambda P(F_{k-1}^s)P(H-v) \\
&= \frac{P(G)}{(\lambda - r)}\lambda^{k-1-(s+1)}\left[P(H)\right]^{s-1}\begin{bmatrix} P(H)\left\{\lambda(\lambda-r) - p(k-s)\right\} \\ -sp\lambda P(H-v)\end{bmatrix} P(H-v)
\end{aligned}$$

$$+\frac{P(G)}{(\lambda-r)}\lambda^{k-1-(s+1)}\left[P\left(H\right)\right]^{s-1}\begin{bmatrix}P\left(H\right)\left\{\lambda\left(\lambda-r\right)-p\left(k-1-s\right)\right\}\\ -sp\lambda P\left(H-v\right)\end{bmatrix}P\left(H\right)$$

$$-\lambda P\left(H-v\right)\frac{P(G)}{(\lambda-r)}\lambda^{k-(s+2)}\left[P\left(H\right)\right]^{s-1}\begin{bmatrix}P\left(H\right)\left\{\lambda\left(\lambda-r\right)-p\left(k-1-s\right)\right\}\\ -sp\lambda P\left(H-v\right)\end{bmatrix}$$

$$=\frac{P(G)}{(\lambda-r)}\lambda^{k-(s+2)}\left[P\left(H\right)\right]^{s}\begin{bmatrix}P\left(H\right)\left\{\lambda\left(\lambda-r\right)-p\left(k-(s+1)\right)\right\}\\ -\left(s+1\right)p\lambda P\left(H-v\right)\end{bmatrix}$$

Thus, the theorem is true for $t = s+1$. Hence by mathematical induction the theorem follows. □

Corollary 5.1.

$$P\left(k *_G H\right) = P\left(F_k^k\right) = \frac{P(G)}{(\lambda-r)}\left[P\left(H\right)\right]^{k-1}\left[P\left(H\right)\left(\lambda-r\right)-pkP\left(H-u\right)\right].$$

We shall now use these theorems to construct infinite families of new integral graphs.

Construction 1. *Let $G = K_4 - e$ rooted at v, where v is any of the two non-adjacent vertices of G. Then, by Theorem 5.1, G_v^k is integral if and only if $8k+9$ is a perfect square.*

Illustration:

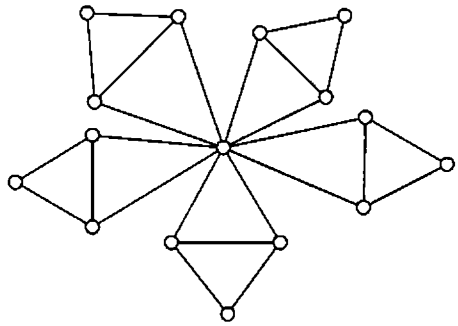


Figure 5.3: $G = K_4 - e,\ k = 5$ with spectrum$[-3, -1^9, 0, 2^4, 4]$

Construction 2. *Let $G = K_{m,n}$ with any vertex v in the n vertex set as a root. Then, G_v^k is integral if and only if both $m(n-1)$ and $m(n-1) + mk$ are perfect squares.*

Example: For $m = t$; $n = t + 1$ and $k = 3t$, G_v^k is integral.

Illustration:

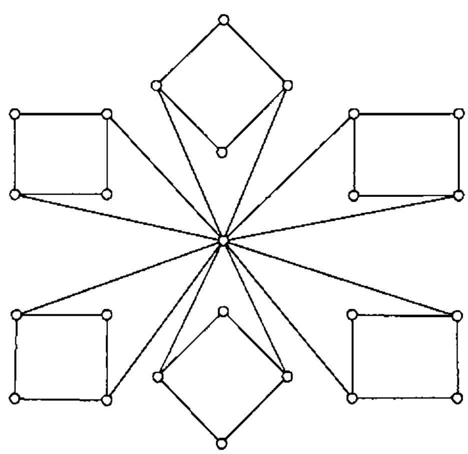


Figure 5.4: $G = K_{2,3},\ k = 6$ with spectrum $[-4, -2^5, 0^{13}, 2^5, 4]$.

Construction 3. *Let G be any $r-$ regular integral graph of order p and H be K_{r+2}. Then, $k *_G H$ is integral if and only if the roots of $(\lambda - r - 1)(\lambda + 1) - pk = 0$ are integers. That is if and only if $(r+2)^2 + 4pk$ is a perfect square.*

Illustration:

Figure 5.5: $G = K_3,\ r = 2,\ H = K_4,\ k = 4$ $\quad$ $G = C_4,\ r = 2,\ H = K_4,\ k = 3$

Some more integral graphs

We define the following operations on a graph G.

Operation 1. *Corresponding to each edge of G introduce a vertex and make it adjacent to the vertices incident with it. Now, introduce k isolated vertices and make all of them adjacent to all the vertices of G.*

Operation 2. *Form the subdivision graph of G (Definition 15). Introduce k vertices and make all of them adjacent to all the vertices of G.*

Operation 3. *Form the subdivision graph of G and add a pendant edge at each vertex of G. Introduce k vertices and make all of them adjacent to all the vertices of G.*

Operation 4. *Take two copies of the $t-$ subdivision graph $S(G)_t$ of G (Definition 35) and join every vertex of G in one of the copies to all the vertices of G in the other copy.*

Theorem 5.3. *Let G be a connected $r-$ regular (p, q) graph with an adjacency matrix A, incidence matrix R and spectrum $\{r, \lambda_2, \lambda_3, ..., \lambda_p\}$. Let F_i be the graph obtained from G by Operation i, $i = 1$ to 4. Then,*

$$spec(F_1) = \begin{pmatrix} 0 & \frac{r\pm\sqrt{r^2+4(pk+2r)}}{2} & \frac{\lambda_i\pm\sqrt{\lambda_i^2+4(\lambda_i+r)}}{2} \\ k+q-p & 1 & 1 \end{pmatrix}$$

$$spec(F_2) = \begin{pmatrix} 0 & \pm\sqrt{(pk+2r)} & \pm\sqrt{(\lambda_i+r)} \\ k+q-p & 1 & 1 \end{pmatrix}$$

$$spec(F_3) = \begin{pmatrix} 0 & \pm\sqrt{(pk+2r+1)} & \pm\sqrt{(\lambda_i+r+1)} \\ k+q & 1 & 1 \end{pmatrix}$$

$$spec\,(F_4) = \begin{pmatrix} 0 & \frac{p\pm\sqrt{p^2+8rt}}{2} & \frac{-p\pm\sqrt{p^2+8rt}}{2} & \pm\sqrt{t\,(\lambda_i+r)} \\ 2(qt-p) & 1 & 1 & 2 \end{pmatrix}, i = 2 \text{ to } p$$

Proof. The proof follows from the Table 1 which gives the adjacency matrix and characteristic polynomial of F_i, $i = 1$ *to* 4 using Lemmas 1.2, 1.4 and 1.7.

Table 1

Graph	$A(F_i)$	$P(F_i)$
F_1	$\begin{bmatrix} A & R & J_{p\times k} \\ R^T & 0 & 0 \\ J_{k\times p} & 0 & 0 \end{bmatrix}$	$\lambda^{q+k-p}\prod_{i=1}^{p}[\lambda^2-\lambda_i\lambda-(kJ+\lambda_i+r)]$
F_2	$\begin{bmatrix} 0 & R & J_{p\times k} \\ R^T & 0 & 0 \\ J_{k\times p} & 0 & 0 \end{bmatrix}$	$\lambda^{q+k-p}\prod_{i=1}^{p}[\lambda^2-(kJ+\lambda_i+r)]$
F_3	$\begin{bmatrix} 0 & R & I & J_{p\times k} \\ R^T & 0 & 0 & 0 \\ I & 0 & 0 & 0 \\ J_{k\times p} & 0 & 0 & 0 \end{bmatrix}$	$\lambda^{q+k}\prod_{i=1}^{p}[\lambda^2-(kJ+\lambda_i+r+1)]$
F_4	$\begin{bmatrix} X & Y \\ Y & X \end{bmatrix}$	$\lambda^{2(qt-p)}\prod_{i=1}^{p}\left\{\begin{array}{l}[\lambda(\lambda-J)-t(\lambda_i+r)] \\ \times[\lambda(\lambda+J)-t(\lambda_i+r)]\end{array}\right\}$

where $X = \begin{bmatrix} 0_p & J_{1\times t}\otimes R \\ J_{t\times 1}\otimes R^T & 0_{qt} \end{bmatrix}$ and $Y = \begin{bmatrix} J_p & 0_{p\times qt} \\ 0_{qt\times p} & 0_{qt} \end{bmatrix}$ $\square$

Examples:

1. $G = K_{n,n}$. F_1 is integral if and only if $n = t^2$, and $k = 2l^2 \pm lt - 1, l \geqslant t,\ t \geq 1$.

2. $G = K_{n,n}$. F_2 is integral if and only if $n = t^2$, and $k = 2h^2 - 1,\ t \geq 1,\ h \geq 1$.

3. $G = K_p$. F_3 is integral when $p = t^2 + 1$, and $k = (t^2+1)h^2 \pm 2th - 1,\ t \geq 1,\ h \geq 1$.

4. $G = K_{n,n}$. F_3 is integral when $n = t^2 - 1$, and $k = 2(t^2 - 1)h^2 \pm 2h - 1,\ t \geq 1,\ h \geq 1$.

5. $G = K_{n,n}$. F_3 is integral when $t = 4n$.

6. $G = K_p$. F_4 is integral when $t = p - 2$.

Theorem 5.4. *Let G be an integral graph with spectrum $\{\lambda_1, \lambda_2, \ldots\ldots, \lambda_p\}$. Then, $splt(G)_t$ is integral if and only if $4t + 1$ is a perfect square.*

Proof. By Definition 36, the adjacency matrix of $splt(G)_t$ can be written as $\begin{bmatrix} A & J_{1\times t} \otimes A \\ J_{t\times 1} \otimes A & 0_{pt} \end{bmatrix}$ so that its characteristic polynomial is $\lambda^{p(t-1)} \prod_{i=1}^{p} [\lambda(\lambda - \lambda_i) - t\lambda_i^2]$ and $spec\,(splt(G)_t) = \begin{pmatrix} \left(\frac{1\pm\sqrt{4t+1}}{2}\right)\lambda_i & 0 \\ 1 & p\,(t-1) \end{pmatrix}$, $i = 1$ *to* p by Lemmas 1.6 and 1.1. Therefore $splt(G)_t$ is integral if and only if $4t + 1$ is a perfect square. $\square$

Illustration:

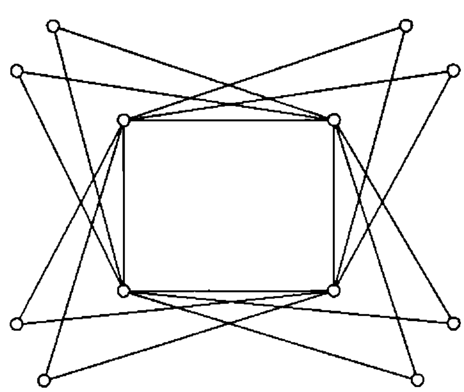


Figure 5.6: $splt(C_4)_2$ with spectrum $[-4, -2, 0^8, 2, 4]$

5.2 Equienergetic integral graphs

In this section we prove the existence of a pair of equienergetic integral graphs of same regularity on every p vertices, $p \equiv 0 (mod\ 4)$. Let G be a graph of order p.

Operation 5. *Take two copies of G on $V = \{v_1, v_2, \ldots, v_p\}$ and $U = \{u_1, u_2, \ldots, u_p\}$ corresponding to the vertices of G. Make u_i adjacent to all the vertices in $\overline{N[v_i]}$ for each $i = 1, 2, \ldots, p$.*

Operation 6. *Take two copies of $\overline{G}$ on $V = \{v_1, v_2, \ldots, v_p\}$ and $U = \{u_1, u_2, \ldots, u_p\}$ corresponding to the vertices of G. Make u_i adjacent to all the vertices in $N(v_i)$ in G for each $i = 1, 2, \ldots, p$.*

Theorem 5.5. *Let G_1 and G_2 be the graphs obtained using Operations 5 and 6. Then, G_1 and G_2 are equiregular and equienergetic.*

Proof. The graphs G_1 and G_2 are $p-1$ regular and of order $2p$. The adjacency matrices of G_1 and G_2 can be written as $\begin{bmatrix} A & \overline{A} \\ \overline{A} & A \end{bmatrix}$ and $\begin{bmatrix} \overline{A} & A \\ A & \overline{A} \end{bmatrix}$ respectively. Then, by Lemmas 1.1 and 1.6, we have

$$spec\,(G_1) = \begin{pmatrix} p-1 & -(p-2r-1) & -1 & 2\lambda_i + 1 \\ 1 & 1 & p-1 & 1 \end{pmatrix}$$

$$spec\,(G_2) = \begin{pmatrix} p-1 & (p-2r-1) & -1 & -(2\lambda_i + 1) \\ 1 & 1 & p-1 & 1 \end{pmatrix}, i = 2 \text{ to } p.$$

Thus, G_1 and G_2 are equienergetic. □

Note: If G is self-complementary $G_1 = G_2$,.

Theorem 5.6. *For every $p \equiv 0 \ (mod\ 4)$, there exists a pair of equienergetic integral graphs.*

Proof. Let $G = CP(n)$. Then, by Lemma 1.11 and Theorem 5.5

$$spec\,(G_1) = \begin{pmatrix} 2n-1 & 2n-3 & -1 & 1 & -3 \\ 1 & 1 & 2n-1 & n & n-1 \end{pmatrix}$$

$$spec\,(G_2) = \begin{pmatrix} 2n-1 & -(2n-3) & -1 & 3 \\ 1 & 1 & 3n-1 & n-1 \end{pmatrix}.$$

Thus, G_1 and G_2 are integral graphs on $4n$ vertices with

$\mathcal{E}(G_1) = \mathcal{E}(G_2) = 2(5n-4)$. Hence the theorem. □

Illustration:

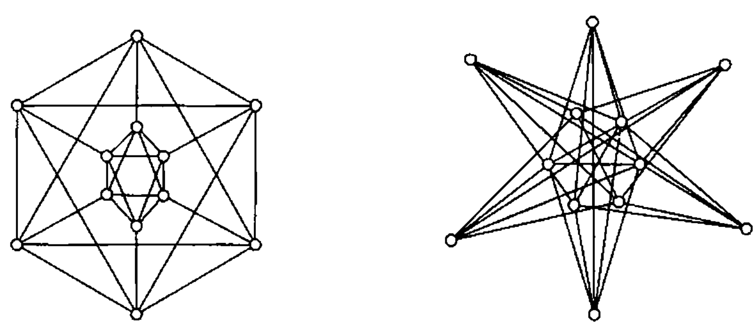


Figure 5.7: Equienergetic integral graphs on 12 vertices with energy 22.

5.3 New integral split graphs

In this section some new integral split graphs are constructed.

We first observe that $splt(K_p)_t$ is an integral split graph if and only if $4t+1$ is a perfect square by Theorem 5.4.

Operation 7. *Let G be a graph on $\{v_1, v_2, \ldots, v_p\}$. Construct $splt(G)_t$ (Definition 36). Then, introduce a set of k isolated vertices and make all of them adjacent to the vertices of G only. The resulting graph is denoted by $[splt(G)_t : k]$.*

Illustration:

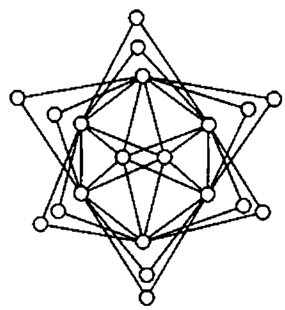


Figure 5.8: $[splt(C_6)_2 : 2]$

Theorem 5.7. *Let G be an $r-$regular integral graph. Then, for $t = h^2 \pm h$, $h \geq 0$ and $k = m[pm \pm lr]$, $l = \sqrt{4t+1}$, $m \geq 1$, $[splt(G)_t : k]$ is integral.*

Proof. The adjacency matrix of $[splt(G)_t : k]$ can be written as
$$\begin{bmatrix} A & J_{1\times t}\otimes A & J_{p\times k} \\ J_{t\times 1}\otimes A & 0_{pt} & 0 \\ J_{k\times p} & 0 & 0_k \end{bmatrix}.$$ Then,

$$spec([splt(G)_t : k]) = \begin{pmatrix} \frac{r\pm\sqrt{(4t+1)r^2+4pk}}{2} & \left(\frac{1\pm\sqrt{4t+1}}{2}\right)\lambda_i & 0 \\ 1 & 1 & p\,(t-1)+k \end{pmatrix}, i = 2\, to\, p,$$

by Lemmas 1.6 ,1.7 and 1.1. Hence the theorem. □

Note: $[splt(K_p)_t : k]$ in an integral split graph.

Illustration:

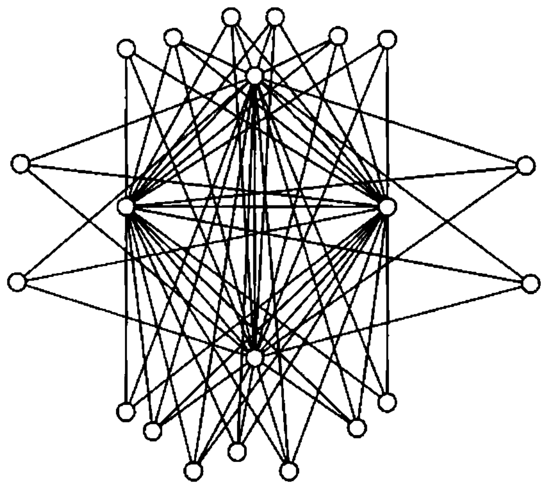


Figure 5.9: $[splt(K_4)_{\mathbf{2}} : 9]$ with spectrum $[-6, -2^3, 0^{13}, 1^3, 9]$

Theorem 5.8. *Let G be an $r-$ regular graph. Then,*

$$spec\,(edsplt(G)_t) = \begin{pmatrix} \frac{r\pm\sqrt{r^2+8rt}}{2} & \frac{\lambda_i\pm\sqrt{\lambda_i^2+4t(\lambda_i+r)}}{2} & 0 \\ 1 & 1 & qt-p \end{pmatrix}, i = 2 \text{ to } p.$$

Proof. By Definition 37, the adjacency matrix of $edsplt(G)_{\mathbf{t}}$ can be written as $\begin{bmatrix} A & J_{1\times t}\otimes R \\ J_{t\times 1}\otimes R^T & 0_{qt} \end{bmatrix}$. Then, by Lemmas 1.6 and 1.1,the theorem follows. □

Note: The split graph $edsplt(K_p)_{\mathbf{p\text{-}1}}$ is integral for each p.

Illustration:

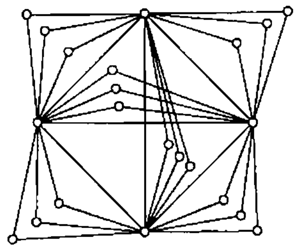


Figure 5.10: $edsplt(K_4)_3$ with spectrum $[-3^4, 0^{14}, 2^3, 6]$.

The following operation extends the operation of attaching $t-$ pendant vertices to each vertex of a regular graph G, defined in [107].

Operation 8. *Let G be a graph on p vertices. Attach t pendant vertices at each vertex of G. Then, introduce k isolated vertices and join each of them to all the vertices of G only. The resulting graph is denoted by $[G^t : k]$.*

Illustration:

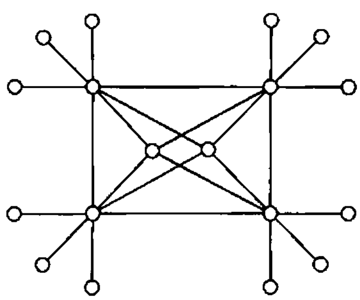


Figure 5.11: $[C_4^3 : 2]$

Theorem 5.9. *Let G be an $r-$regular graph with $spec(G) = \{r,\ \lambda_2,\ \ldots\ldots,\ \lambda_p\}$. Then,* $spec[G^t : k] = \begin{pmatrix} \frac{r\pm\sqrt{r^2+4t+4pk}}{2} & \frac{\lambda_i\pm\sqrt{\lambda_i^2+4t}}{2} & 0 \\ 1 & 1 & p\,(t-1)+k \end{pmatrix}$, $i = 2$ *to* p.

Proof. The adjacency matrix of $[G^t : k]$ can be written as $\begin{bmatrix} A & J_{1\times t}\otimes I & J_{n\times k} \\ J_{t\times 1}\otimes I & 0_{nt} & 0 \\ J_{k\times n} & 0 & 0_k \end{bmatrix}$. Then, by Lemmas 1.1, 1.6 and 1.7 the theorem follows. □

Note: The split graph $[K_p^t : k]$ is integral split if and only if both $4t+1$ and $(p-1)^2 + 4t + 4pk$ are perfect squares.

The following are some values of t and k which gives infinite families of integral split graphs.

- $t = 2,\ k = \frac{p(l^2-1)+2(1\pm 3l)}{4},\ l\ odd.$
- $t = p^2 + p;\ k = p + 1,\ p \geq 2.$

Illustration:

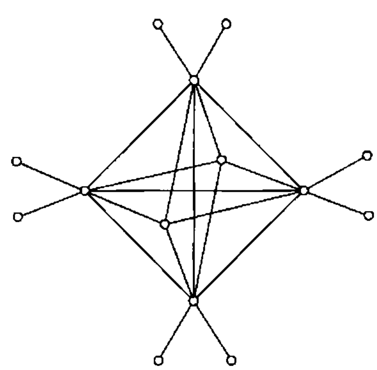


Figure 5.12: $[K_4^2 : 2]$ with spectrum $[-2^4, 0^6, 1^3, 5]$

Chapter 6

Türker equivalent graphs

In this chapter some families of Türker equivalent graphs are constructed.

6.1 Some classes of Türker equivalent graphs

It is known [45] that isomorphic graphs are Türker equivalent.

Theorem 6.1. *Let* $\mathcal{G} = \{G/G \text{ is an } r- \text{ regular graph, } r \geq 3\}$ *and* $\mathcal{F}_k = \{L^k(G),\ k \geq 2/G \in \mathcal{G}\}$. *Then, for each* k *the family* $\mathcal{F}_k$ *is Türker equivalent.*

Proof. Let G be an $r-$ regular graph on p vertices, $r \geq 3$. Then, by Lemmas 1.15

and Equation (1.2), for the family $L^2(G)$ we have the following.

$$Y = pr(r-1)\sqrt{\frac{2r-3}{2} - 4\left(\frac{r-2}{r-1}\right)^2}$$
$$\tan\alpha = \frac{2(r-1)}{5r-9}\sqrt{\frac{2r-3}{2} - 4\left(\frac{r-2}{r-1}\right)^2}$$
$$\tan\beta = \frac{2(r-1)}{2r^2-r-5}\sqrt{\frac{2r-3}{2} - 4\left(\frac{r-2}{r-1}\right)^2}.$$

Here $\tan\alpha$ and $\tan\beta$ are independent of p , the number of vertices of G and depends only on r, its regularity and hence α and β are the same for the family $L^2(G)$. Since $L^k(G) = L^2(H)$ for some regular graph H, this can be extended to the family $L^k(G)$, for $k \geq 3$. □

Theorem 6.2. *Let G be any graph. Let $\mathcal{D}_G = \bigcup_k D^kG$ where D^kG is defined iteratively by $D^0G = G$ and $D^kG = D(D^{k-1}G), k \geq 2$. Then, $\mathcal{D}_G$ is a Türker equivalent family of graphs.*

Proof. Let G be a (p, q) graph with energy $\mathcal{E}$ and Türker angles α, β and θ. Then, by [54], DG, the duplicate graph of G is a $(2p, 2q)$ graph with energy $2\mathcal{E}$.

Let α', β' and θ' be the Türker angles of DG. Then, from Equation (1.2) we have the following,

$$\tan\alpha' = \frac{\sqrt{2\times 2q\times 2p - (2\mathcal{E})^2}}{2p+2\mathcal{E}}$$
$$= \frac{\sqrt{2pq-\mathcal{E}^2}}{p+\mathcal{E}} = \tan\alpha$$
$$\tan\beta' = \frac{\sqrt{2\times 2q\times 2p - (2\mathcal{E})^2}}{2\times 2q+2\mathcal{E}}$$
$$= \frac{\sqrt{2pq-\mathcal{E}^2}}{2q+\mathcal{E}} = \tan\beta$$

Thus, the theorem follows. □

Theorem 6.3. *Let* $\mathcal{F}_k = \left\{L^k(G)/G \text{ is an } r- \text{ regular graph, } r \geq 3,\ k \geq 2\right\}$ *and* $\mathcal{H}_k = \{splt(F_k) \text{ where } F_k \in \mathcal{F}_k\}$*. Then, the family* $\mathcal{H}_k$ *is Türker equivalent for each* k*.*

Proof. Let G be a (p,q) graph and $k = 2$. Then, by [84], $splt(G)$ is a $(2q, 3p)$ graph. Then,

$$\begin{aligned}
N &= \left|V\left[splt\left\{L^2(G)\right\}\right]\right| = 2 \times \left|V\left[L^2(G)\right]\right| \\
&= pr(r-1) \\
M &= \left|E\left[splt\left\{L^2(G)\right\}\right]\right| = 3 \times \left|E\left\{L^2(G)\right\}\right| \\
&= 3 \times \frac{pr(r-1)(2r-3)}{2} \\
\mathcal{E} &= \mathcal{E}\left[splt\left\{L^2(G)\right\}\right] = \sqrt{5} \times \mathcal{E}\left\{L^2(G)\right\}, \\
&= 2\sqrt{5}pr(r-2) \text{ by Lemmas } 1.15 \text{ and } 4.1
\end{aligned}$$

Also, $Y = \sqrt{2MN - \mathcal{E}^2} = \sqrt{3p^2r^2(r-1)^2(2r-3) - 20p^2r^2(r-2)^2}$. Thus, the Türker angles are given as follows.

$$\begin{aligned}
\tan\alpha &= \frac{Y}{N+\mathcal{E}} = \frac{\sqrt{3(r-1)^2(2r-3) - 20(r-2)^2}}{(r-1) + 2\sqrt{5}(r-2)}. \\
\tan\beta &= \frac{Y}{2M+\mathcal{E}} = \frac{\sqrt{3(r-1)^2(2r-3) - 20(r-2)^2}}{3(r-1)(2r-3) + 2\sqrt{5}(r-2)}.
\end{aligned}$$

Since $L^k(G) = L^2(H)$ for some regular graph H, the theorem follows. □

Theorem 6.4. *Let* $\mathcal{T}_k = \{D_2(L^k(G))/G \text{ is an } r- \text{ regular graph}, r \geqslant 3, k \geq 2\}$. *Then, the family* $\mathcal{T}_k$ *is Türker equivalent for each* k.

Proof. Let G be a (p, q) graph and $k = 2$. Then, by [54], $D_2(G)$ is a $(2p, 4q)$ graph. Assume that G is $r \geq 3$ regular. Then,

$$\begin{aligned}
N &= \left|V\left[D_2\left\{L^2(G)\right\}\right]\right| = 2 \times \left|V\left[L^2(G)\right]\right| = pr(r-1) \\
M &= \left|E\left[D_2\left\{L^2(G)\right\}\right]\right| = 4 \times \left|E\left\{L^2(G)\right\}\right| \\
&= 2pr(r-1)(2r-3) \\
\mathcal{E} &= \mathcal{E}\left[D_2\left\{L^2(G)\right\}\right] = 2 \times \mathcal{E}\left\{L^2(G)\right\} \quad \text{by Lemmas 1.15 and 2.1} \\
&= 4pr(r-2)
\end{aligned}$$

Also, $Y = \sqrt{2MN - \mathcal{E}^2} = 2pr\sqrt{(r-1)^2(2r-3) - 4(r-2)^2}$. Thus, the Türker angles are as follows.

$$\begin{aligned}
\tan\alpha &= \frac{Y}{N+\mathcal{E}} = \frac{2\sqrt{(r-1)^2(2r-3) - 4(r-2)^2}}{5r-9}. \\
\tan\beta &= \frac{Y}{2M+\mathcal{E}} = \frac{\sqrt{(r-1)^2(2r-3) - 4(r-2)^2}}{2\left[(r-1)(2r-3) + (r-2)\right]}.
\end{aligned}$$

Since $L^k(G) = L^2(H)$ for some regular graph H, the theorem follows. □

The following theorems provide some more Türker equivalent graphs, the proof of which are on similar lines.

Theorem 6.5. *Let* $\mathcal{G} = \{G/G \text{ is an } r- \text{ regular graph}\}$ *and* $\mathcal{H} = \{H/H \text{ is an } r'- \text{ regular graph }\}$ *where* $r, r' \geqslant 4$. *Then, the family* $L^t(\mathcal{G}) \times L^s(\mathcal{H})$ *is Türker equivalent for each* $t \geq 2$ *and* $s \geq 2$.

Theorem 6.6. *Let* $\mathcal{G} = \{G/G$ *is an* $r-$ *regular graph,* $r \geq 4\}$,

$\mathcal{F}_k = \{L^k(G), k \geq 2/G \in \mathcal{G}\}$ *and* $\mathcal{R}_k = \{R = F_1 \otimes F_2\ /F_1$ *and* $F_2 \in \mathcal{F}_k\}$. *Then,* $\mathcal{R}_k$ *is Türker equivalent for each* k.

Theorem 6.7. *Let* G *be an* $r-$ *regular graph ,* $r \geq 3$. *The the family* $L^k(G) \otimes K_n$ *is Türker equivalent for each* n *and each* $k \geq 2$.

Theorem 6.8. *Let* G *be an* $r-$ *regular graph,* $r \geq 4$. *Then, the family* $L^k(G) \times C_n$ *is Türker equivalent for each* $n \geq 3$ *and* $k \geq 2$.

6.2 Türker equivalent graphs from some graph operations

In this section we define some operations on a graph G with $V(G) = \{v_1, v_2, ..., v_p\}$.

Operation 1. *Introduce two copies of* G *on* $U = \{u_i\}$ *and* $W = \{w_i\}$ *corresponding to* $V = \{v_i\}$. *Make* u_i *and* w_i *adjacent to all the vertices in* $N(v_i)$ *for each* i, $i = 1$ *to* p . *Then, remove the edges of* G *only.*

Operation 2. *Introduce two copies of* G *on* $U = \{u_i\}$ *and* $W = \{w_i\}$ *corresponding to* $V = \{v_i\}$. *Make* u_i *adjacent to all the vertices in* $N(v_i)$ *and* $N(w_i)$. *Then, make* w_i *adjacent to all the vertices in* $N(v_i)$ *and* $N(u_i)$ *for each* i, $i = 1$ *to* p. *Then, remove the edges of* G *only.*

Operation 3. *Operation 3 as in Chapter 4.*

Operation 4. *Operation 5 as in Chapter 4.*

The graph obtained from G using Operation i is denoted by H_i, $i = 1, 2, 3$ and 4.

Theorem 6.9. *Let G be a graph on p vertices with spectrum $\{\lambda_1, \lambda_2, \ldots, \lambda_p\}$ and H_i, $i = 1, 2, 3$ and 4 be the graphs obtained as above. Then,*

1. $\mathcal{E}(H_1) = 4\mathcal{E}(G)$

2. $\mathcal{E}(H_2) = 2\sqrt{3}\mathcal{E}(G)$

3. $\mathcal{E}(H_3) = \mathcal{E}(H_4) = [2\sqrt{2} + 1]\mathcal{E}(G)$

Proof. The table 1 gives the adjacency matrix,its tensor partition and the eigenvalues of H_i, $i = 1, 2$.

Table 1

Operation	Adjacency Matrix	Eigenvalues
1	$\begin{bmatrix} 0 & A & A \\ A & A & 0 \\ A & 0 & A \end{bmatrix} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \otimes A$	$\{2\lambda_i, \lambda_i, -\lambda_i\}$
2	$\begin{bmatrix} 0 & A & A \\ A & A & A \\ A & A & A \end{bmatrix} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \otimes A$	$\{(1 \pm \sqrt{3})\,\lambda_i, 0\}$

Now, the theorem follows from column 3 of Table 1 and Lemma 4.1. □

Note: $H_3 = H_4$ when G is bipartite.

Theorem 6.10. *Let $\mathcal{G}$ be the collection of all $r-$ regular graphs, $r \geq 3$ and $\mathcal{F}_k = \{L^k(G), k \geq 2/G \in \mathcal{G}\}$. Let $\mathcal{F}_{ki} = \{F_{ki}/F_k \in \mathcal{F}_k\}$,$i = 1, 2, 3$ and 4 as defined by the above operations. Then, each family $\mathcal{F}_{ki}$, $i = 1, 2, 3, 4$ and $k \geq 2$ is Türker equivalent.*

Proof. Let G be an $r-$ regular graph on p vertices, $r \geq 3$ and $k = 2$. Then, by Lemma 1.15 and from the above operations we have the order,size and energy of F_{2i} for $i = 1, 2, 3$ and 4 as given in table 2.

Table 2

i	Order of F_{2i}	Size of F_{2i}	Energy of F_{2i}
1	$\frac{3pr(r-1)(2r-3)}{2}$	$3pr(r-1)$	$8pr(r-2)$
2	$\frac{3pr(r-1)(2r-3)}{2}$	$4pr(r-1)$	$4\sqrt{3}pr(r-2)$
3	$\frac{3pr(r-1)(2r-3)}{2}$	$\frac{7pr(r-1)}{2}$	$2\left(2\sqrt{2}+1\right)pr(r-2)$
4	$\frac{3pr(r-1)(2r-3)}{2}$	$\frac{7pr(r-1)}{2}$	$2\left(2\sqrt{2}+1\right)pr(r-2)$

Now, for each i, the Table 3 gives the three Türker angles.

Table 3

i	$\tan\alpha$	$\tan\beta$
1	$\frac{2\sqrt{18r^3-127r^2+328r-283}}{6r^2+r-23}$	$\frac{\sqrt{18r^3-127r^2+328r-283}}{2(7r-11)}$
2	$\frac{2\sqrt{18r^3-127r^2+328r-283}}{6r^2+r(8\sqrt{3}-15)-(16\sqrt{3}-9)}$	$\frac{\sqrt{18r^3-127r^2+328r-283}}{4\left[\left(2+\sqrt{3}\right)r-2\left(1+\sqrt{3}\right)\right]}$
3	$\frac{4\sqrt{6r^3-33r^2+72r-57}}{\left[6r^2+r\left(8\sqrt{2}-11\right)-\left(16\sqrt{2}-1\right)\right]}$	$\frac{2\sqrt{6r^3-33r^2+72r-57}}{\left[r\left(4\sqrt{2}+9\right)-\left(8\sqrt{2}+11\right)\right]}$
4	$\frac{4\sqrt{6r^3-33r^2+72r-57}}{\left[6r^2+r\left(8\sqrt{2}-11\right)-\left(16\sqrt{2}-1\right)\right]}$	$\frac{2\sqrt{6r^3-33r^2+72r-57}}{\left[r\left(4\sqrt{2}+9\right)-\left(8\sqrt{2}+11\right)\right]}$

Now, from table 3 and since $L^k(G) = L^2(H)$ for some regular graph H, the theorem follows. □

6.3 Conclusion and suggestions for further study

In this thesis we have attempted problems regarding construction of equienergetic pairs of graphs in different families of graphs, construction of graphs having a specific pattern in their spectrum and identification of some Türker equivalent graphs.

We propose the following problems for further study.

- Construction of equiregular equienergetic graphs and equienergetic self-complementary graphs on p vertices for all values of p.
- Construction of equienergetic graphs and deriving energy bounds in some other graph classes such as planar graphs, eulerian graphs, chordal graphs etc.
- New constructions for equienergetic reciprocal and integral graphs.
- Study of the properties of the spectrum and the energy of graphs in relation to other graph parameters such as connectivity, independence number, domination number etc.

Bibliography

[1] R. Albert, H.Jeong, A. L. Barabasi, *Diameter of the world-wide web*, Nature, **401**(1999), 130 - 131.

[2] R. Albert, A. L. Barabasi, *Statistical mechanics of complex networks*, Rev. Mod. Phys., **74**(2002), 47 - 97.

[3] R. Balakrishnan, K. Ranganathan, *A Text Book of Graph Theory*, Springer, (1999).

[4] R. Balakrishnan, *The energy of a graph*, Linear Algebra Appl., **387**(2004), 287 - 295.

[5] A. T. Balaban, *Chemical Applications of Graph Theory*, Academic Press, (1976).

[6] K. Balasubramanian, *Computer generation of the characteristic polynomial of chemical graphs*, J. Comput. Chem., **5** (1984), 387 - 394.

[7] K. Balasubramanian, *The use of frames method for the characteristic polynomials of chemical graphs*, Theoret. Chim. Acta Berl., **65**(1984), 49 - 58.

[8] K. Balińska, D. Cvetković, Z. Radosavljević, S. Simić, D. Stevanović, *A Survey on integral graphs*, Univ. Beograd, Publ. Elektrotehn. Fak. Ser. Mat., **13** (2002), 42 - 65.

[9] R. B. Bapat, *Energy of a graph is never an odd integer*, Bull. Kerala Math. Assoc., **1**(2) (2004), 129 - 132.

[10] S. Barik, S. Pati, B. K. Sarma, *The spectrum of the corona of two graphs*, SIAM J. Discrete Math., **21**(2007), 47-56.

[11] S. Barik, M. Neumann and S. Pati, *On non-singular trees and a reciprocal eigenvalue property*, Linear Multilinear Algebra, **54**(2006), 453 - 465.

[12] L. W. Beineke, R. J. Wilson, *Graph Connections*, Oxford University Press, (1997).

[13] C. Berge, *The Theory of Graphs*, Methuen, (1962).

[14] N. L. Biggs, *Algebraic Graph Theory*, Cambridge University Press, (1974).

[15] N. L. Biggs, E. K. Lloyd, R. J. Wilson, *Graph Theory 1736 - 1936*, Oxford University Press, (1976).

[16] D. Cao, H. Yuan, *Graphs characterized by the second eigenvalue*, J. Graph Theory, **17** (1993), 325 - 331.

[17] A. Chen, A. Chang, W. C. Shiu, *Energy ordering of unicyclic graphs*, MATCH Commun. Math. Comput. Chem., **55**(2006), 95 - 102.

[18] C. A. Coulson, *On the calculation of the energy in unsaturated hydrocarbon molecules*, Proc. Cambridge Phil. Soc., **36** (1940), 201 - 203.

[19] C. A. Coulson, B. OĹeary, R. B. Mallion, *Hückel Theory for Organic Chemists*, Academic Press, (1978).

[20] C. A. Coulson, G. S. Rushbrooke, *Note on the method of molecular orbitals*, Proc. Cambridge Phil. Soc., **36**(1940), 193 - 200.

[21] D. M. Cvetković, *Cubic integral graphs*, Univ. Beograd, Publ Elektrotehn. Fak. Ser. Mat. Fiz., (1975), 107 - 113.

[22] D. M. Cvetković, *Graphs with least eigenvalue -2; a historical survey and recent developments in maximal exceptional graphs*, Linear Algebra Appl., **356** (2002), 189 - 210.

[23] D. M. Cvetković, *Graphs with least eigenvalue -2; the eigenspace of the eigenvalue -2*, Rend. Sem. Mat. Messina Ser.II, **9** (2003), 63 - 86.

[24] D. M. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Applications*, Academic Press, (1980).

[25] D. M. Cvetković, I. Gutman, *The algebraic multiplicity of the number zero in the spectrum of a bipartite graph*, Mat.Vesnik., **24**(1972), 141- 150.

[26] D. M. Cvetković, I. Gutman, *On spectral structure of graphs having the maximal eigenvalue not greater than two*, Publ. Inst. Math. (Beograd) (N.S.), **18**(1975), 39 - 45.

[27] D. M. Cvetković, P. Rowlinson, S. Simić, *Eigenspaces of Graphs*, Cambridge University Press, (1997).

[28] D. M. Cvetković, S. Simić, *On graphs whose second largest eigenvalue does not exceed* $\frac{\sqrt{5}-1}{2}$, Discrete Math., **138** (1995), 213 - 227.

[29] D. M. Cvetković, S. Simić, D. Stevanović, *4-regular integral graphs*, Univ. Beograd, Publ. Elektrotehn. Fak. Ser. Mat., **9**(1998), 89 - 102.

[30] D. M. Cvetković, D. Stevanović, *Graphs with least eigenvalue at least* $-\sqrt{3}$, Publ. Inst. Math. (Beograd) (N.S.), **73** (2003), 39 - 51.

[31] P. J. Davis, *Circulant Matrices*, John Wiley & Sons, (1979).

[32] J. R. Dias, *Properties and relationships of conjugated polyenes having a reciprocal eigenvalue spectrum - dendralene and radialene hydrocarbons*, Cro. Chem. Acta., **77**(2004), 325 - 330.

[33] A. Farrugia, *Self-complementary graphs and generalisations:A comprehensive reference manual*, M.Sc Thesis, University of Malta, (1999).

[34] F. R. Gantmacher, *Applications of the Theory of Matrices* **II**, Interscience, (1959).

[35] C. D. Godsil, G. Royle, *Algebraic Graph Theory*, Springer, (2001).

[36] M. C. Golumbic, *Algorithmic Graph Theory and Perfect Graphs*, Academic Press, (1980).

[37] A. Graovac, I. Gutman, N. Trinajstic, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer, (1977).

[38] H.H. Günthard, H.Primas, *Zusammenhang von graphentheorie und MO-Theorie von molekeln mit systemen konjugierter bindungen*, Helv. Chim. Acta, **39**(1956), 1645 - 1653.

[39] I. Gutman, *The energy of a graph*, Ber. Math. Statist. Sekt. Forschungszenturm Graz., **103** (1978), 1 - 22.

[40] I. Gutman, *On the Türker angles in the theory of total $\pi-$ electron energy*, Turk. J. Chem., **22** (1998), 399 - 402.

[41] I. Gutman, *The energy of a graph: old and new results*, In: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), Algebraic Combinatorics and Applications, Springer, (2000), 196 - 211.

[42] I. Gutman, *Topology and stability of conjugated hydrocarbons: The dependence of total π-electron energy on molecular topology*, J. Serb. Chem. Soc., **70** (2005), 441 - 456.

[43] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, (1986).

[44] I. Gutman, L. Türker, *Approximating the total π-electron energy of benzenoid hydrocarbons: Some new estimates of $(n;m)$-type*, Indian J.Chem., **32 A** (1993), 833 – 836.

[45] I. Gutman, L.Türker, *Angle of graph energy - A spectral measure of resemblance of isomeric molecules*, Indian J.Chem., **42 A** (2003), 2698 - 2701.

[46] I. Gutman, L. Türker, *Estimating the angle of total π-electron energy*, J. Mol. Struct., **668** (2004), 119 - 121.

[47] P. Hansen, H. Mèlo, D. Stevanović, *Integral complete split graphs.*, Univ. Beograd, Publ. Elektrotehn. Fak. Ser. Mat., **13** (2002), 89 - 95.

[48] F. Harary, *Graph Theory*, Narosa, (2000).

[49] F. Harary, A. J. Schwenk, *Which graphs have integral spectra?* Graphs Combin., (1974), 45 - 51.

[50] Y. Hou, *Unicyclic graphs with minimal energy*, J. Math. Chem., **29**(2001), 163 – 168.

[51] Y. Hou, *Unicyclic graphs with maximal energy*, Linear Algebra Appl., **356**(2002), 27 - 36.

[52] B.A. Huberman, *The Laws of the Web*, MIT Press, (2001).

[53] E.Hückel, *Quantentheoretische beitrage zum benzolproblem*, Z.Phys., **70**(1931), 204 - 286.

[54] G. Indulal, A. Vijayakumar, *On a pair of equienergetic graphs*, MATCH Commun. Math. Comput. Chem., **55**(2006), 83 - 90.

[55] G. Indulal, A. Vijayakumar, *Energies of some non-regular graphs*, J. Math. Chem., (to appear). *www.springerlink.com/content/y5x275l582386qn3*

[56] G. Indulal, A. Vijayakumar, *Equienergetic self-complementary graphs*, Czechoslovak Math. J.,(to appear).

[57] G. Indulal, A. Vijayakumar, *Some new integral graphs*, Applicable Analysis and Discrete Mathematics, (to appear).
Available online at *http : //pefmath.etf.bg.ac.yu/accepted/rad574.pdf*

[58] G. Indulal, A. Vijayakumar, *Türker equivalent graphs*, (Communicated).

[59] G. Indulal, A. Vijayakumar, *Reciprocal graphs*, (Communicated).

[60] J.M. Kleinberg, *Navigation in a small world*, Nature, **406**(2000), 845.

[61] D. König, *Theorie der Endlichen und Unendlichen Graphen*, Leipzig(1936).

[62] J. Koolen, V. Moulton, *Maximal energy graphs*, Adv. Appl. Math., **26**(2001), 47 - 52.

[63] J. Koolen, V. Moulton, *Maximal energy bipartite graphs*, Graphs Combin., **19**(2003), 131 - 135.

[64] M. Lepović, *On integral graphs which belong to the class $\overline{\alpha K_{a,b}}$*, Graphs Combin., **19**(2003), 527 - 532.

[65] M. Lepović, *On integral graphs which belong to the class $\overline{\alpha K_a \cup \beta K_b}$*, J. Appl. Math. Comput., **14**(2004), 39 - 49.

[66] M. Lepović, *On integral graphs which belong to the class $\overline{\alpha K_a \cup \beta K_{b,b}}$*, Discrete Math., **285**(2004), 183 - 190.

[67] F. Li, B. Zhou, *Minimal energy of bipartite unicyclic graphs with a given bipartition*, MATCH Commun. Math. Comput. Chem., **54** (2005), 379 - 388.

[68] X. L. Li, G. N. Lin, *On integral trees problems*, Kexue Tongbao, **33**(1988), 802 - 806.

[69] W. Lin, X. Guo, H. Li, *On the extremal energies of trees with a given maximum degree*, MATCH Commun. Math. Comput. Chem., **54**(2005), 363 - 378.

[70] B. Mandal, M. Banerjee, A. K. Mukherjee, *Wiener and Hosoya indices of reciprocal graphs*, Mol. Phys., **103**(2005), 2665 - 2674.

[71] B. J. McClelland, *Properties of the latent roots of a matrix:the estimation of $\pi-$ electron energy*, J. Chem. Phys., **54(2)**(1971), 640 - 643.

[72] M. E. J. Newman, *The structure and function of complex networks*, SIAM Rev., **45**(2003), 167 - 256.

[73] S. Nikolić, N. Trinajstić, M. Randić, *Wiener index revisited*, Chem. Phys. Lett., **33**(2001), 319 - 321.

[74] O.Ore, *Theory of Graphs*, Amer. Math. Soc., Providence, (1962).

[75] M. Petroviċ, *On graphs with exactly one eigenvalue less than 1*, J. Combin. Theory Ser. B, **52** (1991), 102 - 112.

[76] M. Petroviċ, *On graphs whose second largest eigenvalue does not exceed* $\sqrt{2}-1$, Univ. Beograd, Publ. Elektrotehn. Fak. Set. Mat., **4** (1993), 70 - 75.

[77] H. S. Ramane, H. B. Walikar, S. B. Rao, B. D. Acharya, I. Gutman, P. R. Hampiholi, S. R. Jog, *Equienergetic graphs*, Kragujevac. J. Math., **26** (2004), 5 - 13.

[78] M. Randic, *On evaluation of the characteristic polynomial for large molecules*, J. Comput. Chem., **3** (1982), 421 - 435.

[79] M. Randić, X. Guo, T. Oxley, H. K. Krishnapriyan, *Wiener matrix:Source of novel graph invarients*, J. Chem. Inf. Comp. Sci., **33(5)**(1993), 709 - 716.

[80] F. S. Roberts, *Discrete Mathematical Models with Application to Social, Biological and Environmental Problems*, Prentice - Hall, (1976).

[81] M. Roitman, *An infinite family of integral graphs*, Discrete Math., **52**(1984), 313 - 315.

[82] H.Sachs, *Beziehungen zwischen den in einem graphen enthaltenen kreisen und seinem charakteristischen polynom.*, Ibid., **11**(1963), 119 - 134.

[83] E. Sampathkumar, *On duplicate graphs*, J. Indian Math. Soc., **37**(1973), 285 - 293.

[84] E. Sampathkumar, H. B. Walikar, *On the splitting graph of a graph*, Karnatak Univ. J. Sci., **35/36** (1980–1981), 13 - 16.

[85] J. Sarkar, A. K. Mukherjee, *Graphs with reciprocal pairs of eigenvalues*, Mol. Phys., **90** (1997), 903 - 907 .

[86] A. J. Schwenk, *Computing the characteristic polynomial of a graph*, In: R. A. Bari, F. Harary, (Eds.), Graphs Combin., Lecture Notes in Mathematics, **406**(1974), 153 - 172.

[87] A. J. Schwenk, *Exactly thirteen connected cubic graphs have integral spectra*, In: Y. Alavi, D. Lick(Eds.), Proceedings of the International Graph Theory Conference at Kalamazoo, Springer,(1976).

[88] A. J. Schwenk, *On the eigenvalues of a graph*, In: L. W. Beineke, R. J. Wilson (Eds.), Selected Topics in Graph Theory, Academic Press, (1979), 307 - 336.

[89] I. Sciriha, S. Fiorini, *On the characteristic polynomial of homeomorphic images of a graph*, Discrete Math. **174** (1997), 293 - 308.

[90] I. Shparlinski, *On the energy of some circulant graphs*, Linear Algebra Appl., **414** (2006), 378 - 382.

[91] J. H. Smith, *Some properties of the spectrum of a graph*, In:R. K. Guy et.al (Eds.) Combinatorial structures and their applications, Gordon and Breach, (1970), 403 - 406.

[92] J. M. Steele, *The Cauchy-Schwarz Master Class*, Cambridge University Press, (2004).

[93] D. Stevanović, *When is NEPS of graphs connected?*, Linear Algebra Appl., **301**(1999), 137 - 144.

[94] D. Stevanović, I. Stanković, *Remarks on hyperenergetic circulant graphs*, Linear Algebra Appl., **400**(2005), 345 - 348.

[95] D. Stevanović, *Energy and NEPS of graphs*, Linear Multilinear Algebra, **53**(2005), 67 - 74.

[96] N. Trinajstić, *Chemical Graph Theory*, CRC press, (1992).

[97] L. Türker, *An approximate method for the estimation of total $\pi-$ electron energies of alternant hydrocarbons*, MATCH Commun. Math. Comput. Chem., **28**(1992), 261-276.

[98] L. Türker, *A novel total $\pi-$ electron energy formula for alternant hydrocarbons - Angle of total $\pi-$ electron energy*, MATCH Commun. Math. Comput. Chem., **30** (1994), 243 - 252.

[99] L. Türker, *Isomerism in the class of alternant hydrocarbons*, J. Mol. Struct., **584**(2002), 183 - 187.

[100] H. B. Walikar, H. S. Ramane, P. R. Hampiholi, *On the energy of a graph*, In: R. Balakrishnan, H. M. Mulder, A. Vijayakumar(Eds.), Graph Connections, Allied Publishers, (1999), 120-123.

[101] H. B. Walikar, H. S. Ramane, *Energy of some cluster graphs*, Kragujevac J. Sci., **23**(2001), 51 - 62.

[102] H. B. Walikar, I. Gutman, P. R. Hampiholi, H. S. Ramane, *Non-hyperenergetic graphs*, Graph Theory Notes N. Y., **51**(2001), 14 - 16.

[103] L. G. Wang, X. L. Li, R. Y. Liu, *Integral trees with diameter 6 or 8*, Electron. Notes Discrete Math., (1999).

[104] L. G. Wang, X. L. Li, *Some new classes of integral trees with diameters 4 and 6*, Australas. J. Combin., **21** (2000), 237 - 243.

[105] L. G. Wang, X. L. Li, S. G. Zhang, *Construction of integral graphs.* Appl. Math. J. Chinese Univ. Ser. B, **15** (2000), 239 - 246.

[106] L. G. Wang, X. L. Li, X. J. Yao, *Integral trees with diameter 4, 6 and 8*, Australas. J. Combin., **25**(2002), 29 - 44.

[107] L. G. Wang, *Integral Trees and Integral Graphs*, Ph.D. Thesis, University of Twente, (2005).

[108] M. Watanabe, *Note on integral trees*, Math. Rep. Toyama Univ., **2** (1979), 95 - 100.

[109] A. Yu, M. Lu, F. Tian, *New upper bounds for the energy of graphs*, MATCH Commun. Math. Comput. Chem., **53**(2005), 441 - 448.

[110] W. Yan, L. Ye, *On the maximal energy and the Hosoya index of a type of trees with many pendant vertices*, MATCH Commun. Math. Comput. Chem., **53**(2005), 449 - 459.

[111] W. Yan, L. Ye, *On the minimal energy of trees with a given diameter*, Appl. Math. Lett., **18** (2005), 1046 - 1052.

[112] D.L. Zhang, H.W. Zhou, *On some classes of integral graphs*, Guangxi Sciences, **10**(2003), 165 - 168.

[113] B. Zhou, *Energy of a graph*, MATCH Commun. Math. Comput. Chem., **51**(2004), 41-49.

[114] B. Zhou, *Lower bounds for energy of quadrangle free graphs*, MATCH Commun. Math. Comput. Chem., **55**(2006), 91 - 94.

[115] B. Zhou, F. Li, *On minimal energies of trees of a prescribed diameter*, J. Math. Chem., (2006), 465 - 473.