ST. GREGORIOS COLLEGE KOTTARAKARA

Student’s Project-PG

2023-2024

Acanthus ilicifolius Leaf Extract Mediated Synthesis Of Tin Oxide Nanoparticles

Project report submitted to the University of Kerala In partial fulfillment of the requirements for the award of the Degree of

MASTER OF SCIENCE IN PHYSICS

By

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This is to certify that the dissertation entitled **"*Acanthus ilicifolius* Leaf Extract Mediated Synthesis Of Tin Oxide Nanoparticles"** submitted to the **University of Kerala** in partial fulfillment of the requirement for the award of the degree of **MASTER OF SCIENCE IN PHYSICS** is a record of original research work done by **V R Vibinraj** during the period 2022-2024, under my guidance at St.Gregorios College, Kottarakara.

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A STUDY ON MIGRATION OF STUDENTS FROM KERALA FOR ABROAD STUDIES WITH SPECIAL REFERENCE TO KOLLAM DISTRICT

PROJECT REPORT

Submitted to the University of Kerala in partial fulfillment of the requirements for the award of degree of

MASTER OF COMMERCE

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DIVERSITY AND DISTRIBUTION OF GASTROPODS AND BIVALVES IN ASHTAMUDI LAKE, KERALA, SOUTH INDIA

Dissertation submitted to the University of Kerala in partial fulfillment of the requirements

for the degree of

Master of Science in Zoology, with a specialization in Biosystematics and Biodiversity

By

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This is to certify that this project entitled "Diversity and Distribution of Gastropods and Bivalves in Ashtamudi Lake, Kerala, South India" is an authentic record of work carried out by Devika B,Final year M.Sc. Zoology student under my guidance and supervision and no part of this work has been presented for any other degree or diploma.

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Comparative Study on the Anti-Inflammatory Property of Carnosic Acid, a Phytochemical from *Rosmarinus officinalis* with a Commonly Used Anti-Inflammatory Drug Ibuprofen Using *In silico* Analysis

A dissertation submitted to the University of Kerala in partial fulfillment of the requirements for the Award of degree of Master of Science in Chemistry

Master of Science in Chemistry

BY

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A STUDY ON BITOPOLOGICAL SPACE

Dissertation submitted to the University of kerala in partial fulfillment of the requirements for the award of the

Degree of Master of Science

In

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By

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M.Sc.MATHEMATICS

(2022-2024)

A STUDY ON ENERGY OF GRAPHS

A STUDY ON ENERGY OF GRAPHS

Dissertation submitted to the University of Kerala

in partial fulfillment of the requirements for the award of the

Degree of Master of Science

In

Mathematics

By

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KOTTARAKARA HELANA ELSA PRINCE

Date :

ABSTRACT

Let G be a graph, the energy of graphs is the sum of the absolute values of the eigen value of its adjacency matrix.In this paper we characterize graphs having the maximum energy among all graphs with n vertices.Also we know that complete graph having maximum energy.But various families of hyperenergetic graphs which have an energy larger than the complete graphs.The energy of a graph on n vertices is atmost $\frac{n}{2}\left(1+\sqrt{n}\right)$ if and only if G is strongly regular graph with parameters.This enables to find an infinite family of maximal energy graphs.Using Hadamard matrix, we can find maximum energy graph for every positive integer.Also providing an upper bound for the energy, which is sharp for every special values of n and this bound is achieved for all even squares.For n that is not a square of even number this bound is not sharp, the problem of maximal energy remains open in general case.The method developed here provides a way to improve the upper bound for energy for arbitrary n.

Contents

INTRODUCTION

The energy of a graph is a concept that arose in theoretical chemistry.In mathematics, the energy of graphs is the sum of the absolute values of the eigen value of its adjacency matrix.All graphs considered in this paper are finite, simple and undirected.Here we discuss to characterize graphs having the maximal energy among all graphs with n vertices.

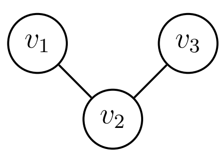
This paper consist of three chapter.First chapter deals with the basic concepts of the energy of graphs.Second chapter gives the idea of energy of graphs with orthogonal matrix. And also discuss graphs having energy larger than complete graphs called hyperenergetic graphs.Third chapter consist of strongly regular graphs with certain parameters is called maximal energy graphs.This enables to find an infinite family of maximal energy graph.The maximal energy graphs are essentially the same objects as certain hadamard matrix.Thus it provides a upper bound for the energy.

Chapter 1

PRELIMINARIES

Definition 1.0.1. *A graph G consist of a finite non-empty set V of objects called vertices and a set E of two element subsets of V of objects called edges. The set V and E are the vertex set and edge set of G respectively.*

Example 1.0.2. $V = \{v_1, v_2, v_3\}, E = \{(v_1, v_2), (v_2, v_3)\}$



Definition 1.0.3. *A simple graph is an unweighted, undirected graph containing no graph loops or multiple edges. A simple graph may be either connected or disconnected.*

Definition 1.0.4. *Let S_n be the family of simple graphs with n vertices $v_1, v_2, \ldots, v_n$. Adjacency matrix $A = A(G)$ of a graph $G \in S_n$ is a square matrix of order n whose entry in the i^{th} row and j^{th} coloumn is defined as :*

$$a_{ij} = \begin{cases} 1 & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent.} \\ 0 & \text{otherwise} \end{cases}$$

Definition 1.0.5. *For a graph $G \in S_n$ with adjacency matrix, the characteristic polynomial of a graph is the characteristic polynomial of the adjacency matrix:*

$$\phi\big(G\big) = \phi\big(G, \lambda\big) = det\big(\lambda I - A\big)$$

Its roots are called eigen values.

Definition 1.0.6. *Let G be a graph of order n with energy $E\big(G\big) = \sum_{i=1}^{n} |\lambda_i|$. The set $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ is the spectrum of G and denoted by $SpecG$.*

Definition 1.0.7. *A symmetric matrix is a square matrix that is equal to its transpose,*

$$A \text{ is symmetric} \Leftrightarrow A = A^T$$

Example 1.0.8. A= $\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$

$$Transpose\ of\ A,\ A^T = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$A = A^T$$

Definition 1.0.9. *A square matrix A is said to be orthogonal matrix if the product of the matrix A and its transpose A^T is an identity matrix.ie,*

$$AA^T = A^T A = I$$

Example 1.0.10. $A = \begin{bmatrix} cos\alpha & 0 & sin\alpha \\ 0 & 1 & 0 \\ -sin\alpha & 0 & cos\alpha \end{bmatrix}$ is orthogonal.

$$A = \begin{bmatrix} cos\alpha & 0 & sin\alpha \\ 0 & 1 & 0 \\ -sin\alpha & 0 & cos\alpha \end{bmatrix}$$

$$A^T = \begin{bmatrix} cos\alpha & 0 & -sin\alpha \\ 0 & 1 & 0 \\ sin\alpha & 0 & cos\alpha \end{bmatrix}$$

$$AA^T = \begin{bmatrix} cos^2\alpha + sin^2\alpha & 0 & -cos\alpha sin\alpha + cos\alpha sin\alpha \\ 0 & 1 & 0 \\ -sin\alpha cos\alpha + sin\alpha cos\alpha & 0 & sin^2\alpha + cos^2\alpha \end{bmatrix}$$

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

Definition 1.0.11. *A set of vectors form an orthonormal set if all vectors in the set are mutually orthogonal and all of unit length.An orthonormal set which forms a basis is called orthonormal basis.*

Definition 1.0.12. *A matrix P is called orthogonal if its coloumns form an orthonormal set and call a matrix A orthogonally diagonalizable if it is diagonalized by $D = P^{-1}AP$ with P an orthogonal matrix.If A is an $n \times n$ symmetric matrix, then any two eigen vectors that come from distinct eigen values are orthogonal.*

Definition 1.0.13. *In the finite dimensional case, a square matrix P is called* *a projection matrix if it is equal to its square,*

$$P^2 = P$$

Definition 1.0.14. *A square matrix P is called orthogonal projection matrix if $P^2 = P = P^T$ for a real matrix and respectively $P^2 = P = P^*$ for a complex matrix, where P^T denotes the transpose of P and P^* denote adjoint.*

Line Graph

A graph with p vertices q edges will referred to as (p, q) graph. Let G be a (p, q) graph, the line graph denoted $L(G)$, the graph whose vertices are the edges of G.The number of vertices and edges of $L(G)$ be n and m respectively. The degree of the vertices of G are $\delta_1, \delta_2, \ldots, \delta_p$.

Then

$$n = q \;:\; m = \frac{1}{2}\sum_{i=1}^{p} \delta_i^2 - q \tag{1.1}$$

Let $D(G) = diag(\delta_1, \delta_2, \ldots, \delta_p)$.Also $A(G)$ be the adjacency matrix of G.Then $D(G) + A(G)$ is a non negative definite matrix and its eigen valus are non negative.

Let $\mu_1, \mu_2, \ldots, \mu_p$ be the eigen value of $D(G) + A(G)$, then

$$\sum_{i=1}^{p} \mu_i \;=\; \sum_{i=1}^{p} \delta_i = 2q \tag{1.2}$$

Definition 1.0.15. *A vertex of degree zero is called isolated vertex.*

Definition 1.0.16. *If the vertices of a graph G have same degree, then G is called regular graph.*

Chapter 2

ENERGY OF GRAPHS

Let G be a graph, the energy of graphs is the sum of the absolute values of the eigen value of its adjacency matrix. Here we characterize graphs having the maximum energy among all graphs with n vertices. We know that complete graph having maximal energy. But various families of graphs which have an energy larger than the complete graphs. Here we consider the hyperenergetic graphs which have energy larger than the complete graphs

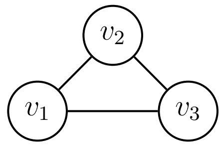
2.1 Energy of Graphs

Definition 2.1.1. *For a graph $G \in S_n$ with adjacency matrix $A = A(G)$ and the eigen values λ_1,$\lambda_2 \ldots \lambda_m$, the* **energy**

$$E = E(G) = E(A) = \sum_{k=1}^{m} |\lambda_k|$$

sum of all eigen values of a graph is zero, $E = 2E^+$, where E^+ denote the sum of positive eigen values.

Example 2.1.2.



Adjacency Matrix Ac_3= $\begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$

Characteristic polynomial=det$(\lambda I - A)$

$$\lambda I - A = \begin{bmatrix} \lambda & -1 & -1 \\ -1 & \lambda & -1 \\ -1 & -1 & \lambda \end{bmatrix}$$

$$\det(\lambda I - A) = \lambda^3 - 3\lambda - 2$$

$$\lambda = -1, -1, 2$$

$$\lambda_1 = -1, \lambda_2 = -1, \lambda_3 = 2$$

Eigen value is $\lambda_1 = -1, \lambda_2 = -1, \lambda_3 = 2$

$$\text{Energy of graph} = \sum_{k=1}^{n} |\lambda_k|$$

$$= |\lambda_1| + |\lambda_2| + |\lambda_3|$$

$$= |-1| + |-1| + |2|$$

$$= 4$$

Definition 2.1.3. *The product of two graphs G_1 and G_2 denoted by $G_1 \times G_2$ is the graph with vertex set $V\big(G_1\big) \times V\big(G_2\big)$ such that two vertices $\big(x_1, x_2\big) \in V\big(G_1 \times G_2\big)$ and $\big(y_1, y_2\big) \in V\big(G_1 \times G_2\big)$ are adjacent if and only if $\big(x_1, y_1\big) \in E\big(G_1\big)$ and $\big(x_2, y_2\big) \in E\big(G_2\big)$*

Definition 2.1.4. *The sum of two graphs* G_1 *and* G_2 *denoted by* $G_1 + G_2$ *is the graph with vertex set* $V(G_1) \times V(G_2)$ *such that* $(x_1, x_2) \in V(G_1 + G_2)$ *and* $(y_1, y_2) \in V(G_1 + G_2)$ *are adjacent if and only if either* $(x_1, y_1) \in E(G_1)$ *and* $x_2 = y_2$ *or* $(x_2, y_2) \in E(G_2)$ *and* $x_1 = y_1$

Lemma 2.1.5. *Let* G_1 *and* G_2 *be two graphs with disjoint vertex sets of order* n_1 *and* n_2 *respectively.Let* λ_i,$i = 1, 2, \ldots, n_1$ *and* λ_j,$j = 1, 2, , \ldots, n_2$ *be the eigen values of the graph* G_1 *and* G_2*.Then the eigen value of* $G_1 \times G_2$ *are* $\lambda_i \lambda_j$, $i = 1, 2, , \ldots, n_1$,$j = 1, 2, , \ldots, n_2$

Lemma 2.1.6. *Let* G_1 *and* G_2 *be two graphs with disjoint vertex sets of order* n_1 *and* n_2 *respectively.Let* λ_i,$i = 1, 2, \ldots, n_1$ *and* λ_j,$j = 1, 2, , \ldots, n_2$ *be the eigen values of the graph* G_1 *and* G_2*.Then the eigen value of* $G_1 + G_2$ *are* $\lambda_i + \lambda_j$, $i = 1, 2, , \ldots, n_1$,$j = 1, 2, , \ldots, n_2$

Lemma 2.1.7. *If an eigen value of a graph is a rational number, then it is an integer.*

Theorem 2.1.8. *The energy of a graph cannot be an odd integer*

Proof. Consider a graph G and λ_1,$\lambda_2 \ldots \lambda_m$ be positive eigen values.Then the fact that sum of all eigen values of any graph is equal to zero

$$E(G) = \sum_{k=1}^{m} |\lambda_k| = 2 \sum_{k=1}^{m} \lambda_k$$

Denote $\lambda_1 + \lambda_2 + \ldots \lambda_m$ by λ

By *lemma* 2.1.5 λ is an eigen value of some graph H isomorphic to the sum of m disjoint copies of the graph G.

Suppose

$$\begin{aligned} E(G) &= q \\ 2\lambda &= q \qquad (2.1) \\ \lambda &= q/2 \end{aligned}$$

If q would be an odd integer,then $q/2$ would be an non integral rational number which is contradiction to *lemma* 2.1.7 □

Theorem 2.1.9. *The energy of a graph cannot be the square root of an odd integer,*

Proof. Consider a graph G and λ_1,$\lambda_2 \ldots \lambda_m$ be positive eigen values.Then the fact that sum of all eigen values of any graph is equal to zero

$$E(G) = \sum_{k=1}^{m} |\lambda_k| = 2\sum_{k=1}^{m} \lambda_k$$

Denote $\lambda_1 + \lambda_2 + \ldots \lambda_m$ by λ

By *lemma* 2.1.5, λ is an eigen value of some graph H isomorphic to the sum of m disjoint copies of the graph G.

By *lemma* 2.1.6, λ^2 is an eigen values of the product of two disjoint copies of the graph H.

Suppose

$$\begin{aligned} E(G) &= \sqrt{q} \\ 2\lambda &= \sqrt{q} \qquad (2.2) \\ \lambda^2 &= q/4 \end{aligned}$$

If q would be an odd integer, then $q/2$ would be an non integral rational number which is contradiction to *lemma* 2.1.7 □

Corollary 2.1.10. *The energy of a graph cannot be the square root of the double of an integer.*

Theorem 2.1.11. *Let r and s be integers such that $r \geq 1$ and $0 \leq s \leq r-1$ and q be an odd integer.Then $E(G)$ cannot be the form $(2^s q)^{\frac{1}{r}}$*

Proof. For $r = 1$ and $s = 0$, *Theorem* 2.1.7 reduces to *Theorem* 2.1.8

For $r = 2$ and $s = 0$, *Theorem* 2.1.7 reduces to *Theorem* 2.1.9

Suppose now that $E\big(G\big) = q^{\frac{1}{r}}$, q is an odd integer

Then

$$2\lambda = q^{\frac{1}{r}}$$
$$\lambda^r = \frac{q}{2^r} \tag{2.3}$$

If q would not be divisible by 2^r,then λ^r would be an non integral rational number,which is contradiction to *lemma* 2.1.7. □

Definition 2.1.12. *The tensor product of two graphs G_1 and G_2 is the graph $G_1 \otimes G_2$ with vertex set $V\big(G_1\big) \times V\big(G_2\big)$ and in which the vertices $\big(u_1, u_2\big)$ and $\big(v_1, v_2\big)$ are adjacent if and only if $u_1v_1 \in E\big(G_1\big)$ and $u_2v_2 \in E\big(G_2\big)$.*

Definition 2.1.13. *The tensor product $A \otimes B$ of the $r \times s$ matrix $A = \big(a_{ij}\big)$ and the $t \times u$ matrix $B = \big(b_{ij}\big)$ is defined as the $rt \times su$ matrix got by replacing each entry a_{ij} of A by the double array $a_{ij}B$.*

Lemma 2.1.14. *If A is matrix of order r with spectrum $\{\lambda_1, \lambda_2 \ldots \lambda_r\}$ and B is a matrix of order s with spectrum $\{\mu_1, \mu_2 \ldots \mu_s\}$ then the spectrum of $A \otimes B$ is $\{\lambda_i\mu_j : 1 \le i \le r, 1 \le j \le s\}$.*

Proof. Let X and Y be eigen vectors corresponding to the eigen values λ and μ of A and B respectively.

Then $AX = \lambda X$ and $BY = \mu Y$

Now for any four matrices P, Q, R and S,

$\big(P \otimes Q\big)\big(R \otimes S\big) = PR \otimes QS,$ whenever the products PR and QS are defined.

Hence $\big(A \otimes B\big)\big(X \otimes Y\big) = AX \otimes BY = \lambda X \otimes \mu Y = \lambda\mu\big(X \otimes Y\big)$. As $\big(X \otimes Y\big)$ is a non-zero vector, $\lambda\mu$ is an eigen value of $\big(A \otimes B\big)$.

Conversely any eigen value of $\big(A \otimes B\big)$ of the form $\lambda_i\mu_j$ for some i and j. To see this we note that

$$\big(A \otimes B\big) = \big(A \otimes I_s\big)\big(I_r \otimes B\big) = \big(I_r \otimes B\big)\big(A \otimes I_s\big)$$

In otherwords $(A \otimes B)$ is a product of two commuting matrices.

Now the spectrum of $(I_r \otimes B)$ is the spectrum of B repeated r times and similar statement applies for the spectrum $(A \otimes I_s)$.

Now if C and D are two commuting matrices of order t,with spectra $\alpha_1, \alpha_2 \ldots \alpha_t$ and $\beta_1.\beta_2 \ldots \beta_t$ respectively, then each of the t eigen values of CD is of the form $\alpha_i\beta_j$ for some i and j.

This proves the result. □

Corollary 2.1.15. *If G_1 and G_2 are any two graphs*

$$E(G_1 \otimes G_2) = E(G_1)E(G_1).$$

Proof. Let the spectra of G_1 and G_2 be $\lambda_1, \lambda_2 \ldots \lambda_r$ and $\mu_1, \mu_2 \ldots \mu_s$ respectively

Then

$$\begin{aligned} E(G_1 \otimes G_2) &= \sum_{i,j} |\lambda_i \mu_j| \\ &= \sum_{i=1}^{r} |\lambda_i| \sum_{j=1}^{s} |\mu_j| \qquad (2.4) \\ &= E(G_1)E(G_2) \end{aligned}$$

□

Corollary 2.1.16. *For any non-trivial graph G, $E(G) > 1$*

Proof. Suppose $E(G) < 1$.Then $E(G \otimes G \otimes G \ldots \otimes G(p\ times)$

$E(G \otimes G \otimes G \ldots \otimes G) = E(G)^p \to 0$ as $p \to \infty$

Hence the graph $G \otimes G \otimes G \ldots \otimes G(p\ times)$ $\to$the totally disconnected graph which is absured.The same arguement show that not all the eigen values of the graph G can be absolute value less than 1.Consequently if $E(G) = 1$,then the absolute value of all the eigen values of G must be less than 1, a contradiction.

□

2.2 Characterization by projectors and orthogonal matrix

The standard basis for $\mathbb{R}^n$ is $E_1, E_2, \ldots, E_n$,where E_j is the element of $\mathbb{R}^n$ with 1 in the j^{th} place and zeros on all other place.If $T : \mathbb{R}^n \to \mathbb{R}^m$ is a linear transformation defined by

$$T\big(E_j\big) = \big(t_{1j}, t_{2j}, \ldots t_{mj}\big) = \sum_{k=1}^{m} t_{kj} E_k$$

If $T : \mathbb{R}^n \to \mathbb{R}^m$ is a linear transformation and β a base in $\mathbb{R}^n$ by $[T]_\beta$ we denote the matrix with respect to the basis β.

Let A be a real symmetric matrix of type $n \times n$ and e_k be orthonormal eigen vectors for A, that is $Ae_k = \lambda k e_k, k = 1, ..., n$ and E_k be the standard basis in $\mathbb{R}_n$. If Q is a linear operator defined by $Q(E_k) = e_k$, then $Q^{-1}AQ = D$, where $D = diag\big(\lambda_1, \lambda_2, ..., \lambda_n\big)$. A real matrix A is symmetric if and only if there is an orthogonal matrix Q such that $Q^1 AQ = D$, where $D = diag\big(\lambda_1, \lambda_2, ..., \lambda_n\big)$. Also $tr\big(A\big) = a_{11} + \ldots + a_{nn} = \sum_i a_{ii}$, where a_{ij} represents the entry on the i^{th} row and j^{th} column of A. Equivalently, the trace of a matrix is the sum of its eigenvalues, making it an invariant with respect to a change of basis. Also $tr\big(Q^1 AQ\big) = tr\big(AQQ^{-1}\big) = trA$.

Theorem 2.2.1. *Suppose that A is a real symmetric matrix with $trA = 0$. If P is an orthogonal projector matrix then $E = E\big(A\big) \geq 2tr\big(AP\big)$; and $E = 2max.tr\big(AP\big)$, where max is taken over all orthogonal projectors P.*

Proof. Let $\big(\lambda_1, \lambda_2, \ldots, \lambda_n\big)$ be eigenvalues of A.

Suppose that $\lambda_1 > \lambda_2 > \ldots > \lambda_p \geq 0$ and $\lambda_k < 0$ for $k > p$.

Let $e = \big(e_1, \ldots, e_n\big)$ be the orthonormal basis of eigenvectors of the matrix A and P_0 be a projector onto the p dimensional space corresponding to non negative eigenvalues.

Then, since $[A]_e = diag\big(\lambda_1, \lambda_2, \ldots, \lambda_n\big)$ and

$tr\big(AP_0\big) = tr\big([A]_e\,[P_0]_e\big)$,

it is clear that $E^+\big(A\big) = tr\big(AP_0\big)$.

We first verify that for any vector $x \in IR_n$

$$(x, Ax) \leqslant (x, AP0x) \tag{2.5}$$

$$\text{If}, x = \sum_{k=1}^{n} t_k e_k,$$

$$\text{then }, Ax = \sum_{k=1}^{n} t_k \lambda_k e_k,$$

$$P_0 x = \sum_{k=1}^{n} t_k e_k \quad \text{and}$$

$$AP_0 x = \sum_{k=1}^{p} t_k \lambda_k e_k.$$

$$\text{Hence }, (x, Ax) = \sum_{k=1}^{n} t_k^2 \lambda_k \quad \text{and}$$

$$(x, AP_0 x) = \sum_{k=1}^{p} t_k^2 \lambda_k$$

therefore, we have $(x, Ax) \leqslant (x, AP0x)$.

Let $\alpha = \big(f_1, f_2, \ldots, f_n\big)$ be an orthonormal basis and

$$Af_k = \sum_{j=1}^{n} a_{kj}, f_j$$

Then

$$trA = \sum_{i=1}^{n} a_{ii} = \sum_{i=1}^{n} \big(f_i, Af_i\big) \tag{2.6}$$

Now let P be an arbitrary orthogonal projection.

Let $\beta_1 = \big(b_1, \ldots, b_r\big)$ be an orthonormal basis for ImP and $\beta_2 = \big(b_{r+1}, \ldots, b_n\big)$ an orthonormal basis for $KerP$.

Then $\beta = \beta_1 \cup \beta_2$ is a basis and

$$P = [P] = \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix},$$

where I_r is a unit matrix.

Since $Pb_i = b_i, i = 1, \ldots, r$ and $Pb_i = 0, i = r+1, \ldots, n$,

we find $APb_i = Ab_i, i = 1, \ldots, r$ and $APb_i = 0, i = r+1, \ldots, n$.

Then, by $\big(2.5\big) and \big(2.6\big)$,

$$\begin{aligned} tr(AP) &= \sum_{i=1}^{r} \big(b_i, Ab_i\big) \\ &\leq \sum_{i=1}^{r} \big(b_i, Ap_0 b_i\big) \\ &\leq tr\big(AP_0\big) = E^+ \end{aligned}$$

□

Lemma 2.2.2. *P is an orthogonal projector if and only if $P = \big(I + O\big)/2$, where O is an orthogonal symmetric matrix.*

Proof. Suppose that O is an orthogonal symmetric matrix and $P = \big(I + O\big)/2$. Then P is symmetric,

$$O = O^t, \; OO^t = I$$

and therefore $O^2 = I$.

Hence $\big(I + O\big)\big(I + O\big) = I + O + O + O^2 = 2\big(I + O\big)$,

that is $P^2 = P$; thus, since P is symmetric, we conclude that P is an orthogonal projector.

Conversely, if P is an orthogonal projector and $O = 2P - I$, then

$O^2 = (2P - I)^2 = 4P - 4P + I = I$, hence $O^2 = I$; moreover, since P is symmetric, O is symmetric, and hence $O^t = O = O^{-1}$, that is O an orthogonal matrix. □

Theorem 2.2.3. *Let G be a simple graph with n vertices and $O^s(n)$ be the family of orthogonal symmetric matrices of type $n \times n$. Then*

$$E(G) \leq \frac{n}{2} + max\frac{1}{2}|O|_1 \leq \frac{n}{2} + \frac{1}{2}n^{\frac{3}{2}},$$

where max is taken over all $O \in O^s(n)$.

It is clear that

$$maxE(G) \leq \frac{n}{2} + max\frac{1}{2}|O|_1 \leq \frac{n}{2} + \frac{1}{2}n^{\frac{3}{2}},$$

where max is taken over all $G \in S_n$.

Proof. If O_n is an orthogonal symmetric matrix with $|o_{ij}| = \sqrt{\frac{1}{n}}, o_{ii} = \sqrt{\frac{1}{n}}$ and $\sum o_{ij} = n$, then O_n is extremal.

Step 1: If $O = [o_{ij}]$ is an orthogonal matrix, then $|O|_1 \leq n^{\frac{3}{2}}$. Since $O = [o_{ij}]$ is an orthogonal matrix $\sum\limits_{i} o_{ik}^2 = 1$, and $\sum\limits_{i,j} |o_{ij}|^2 = n$.

Hence $\big(\sum\limits_{i,j} |o_{ij}|\big)^2 \leq n^2 \sum\limits_{i,j} |o_{ij}|^2 = n^3$.

The equality holds if and only if $|o_{ij}| = c_n$= constant,

i.e.,if and only if $|o_{ij}| = 1/\sqrt{n}$.

Step 2 : If $O = [o_{ij}]$ is an orthogonal matrix, then

$$\sum o_{ij}^{+} \leq \frac{n}{2} + \frac{1}{2}|o|_1 \qquad (2.7)$$

If $P = (I + O)/2$ is a projector and $v_0 = (1, \ldots, 1)$,

then $|Pv_0|^2 = \sum p_{ij} = \frac{n}{2} + \frac{1}{2}\sum o_{ij}$.

Since $|Pv_0|^2 \leq |v_0|^2 = n$,

we find $\sum o_{ij} \leq n$.

Hence, using $\sum o_{ij} = \frac{1}{2}\big(\sum |o_{ij}| + o_{ij}\big)$, we find (2.7).

If A is the symmetric $\big(0,1\big)$-adjacency matrix of G and $AP = [b_{ij}]$,

then $b_{ij} = \sum_k a_{ik} p_{jk}$ and therefore $tr\big(AP\big) = \sum_i b_{ii} = \sum_{i,k=1}^{n} a_{ik} p_{ik}$.

Hence, since A is the symmetric $\big(0,1\big)$-adjacency matrix, $tr\big(AP\big) \leq \sum_{i \neq j} p_{ij}^{+}$.

By *Lemma* 2.2.2, P is an orthogonal projector if and only if $P = \big(I + O\big)/2$,

where O is an orthogonal symmetric matrix.

If $i \neq j, p_{ij} = o_{ij}/2$,

$$
\begin{aligned}
tr(\big(AP\big) \leq \frac{1}{2} \sum_{i \neq j} o_{ij}^{+} \leq & \frac{1}{4} \sum_{i \neq j} o_{ij} + |o_{ij}| \\
\leq & \frac{n}{4} + \frac{1}{4} |o|_1 \\
\leq & \frac{n}{4} + \frac{1}{4} n^{\frac{3}{2}}
\end{aligned}
$$

and therefore

$$max E\big(G\big) \leq \frac{n}{2} + max \frac{1}{2} |O|_1 \leq \frac{n}{2} + \frac{1}{2} n^{\frac{3}{2}}.$$

□

Theorem 2.2.4. *For a graph $G \in S_n$, $E\big(G\big) = max \sum_{i \neq j, \big(i,j\big) \in G} o_{ij}$, where max is taken over all orthogonal symmetric matrices $O = [o_{ij}]$. There is a maximal orthogonal symmetric matrix such that $E\big(G\big) = \sum_{i \neq j, \big(i,j\big) \in G} o_{ij}$*

Proof. Since $O^s\big(n\big)$ is compact, there is a maximal orthogonal symmetric matrix $O = [o_{ij}]$ such that $E\big(G\big) = \sum_{i \neq j, \big(i,j\big) \in G} o_{ij}$ □

2.3 Application

Let us denote

$$o^+ = \sum_{j, i\neq j, \left(i,j\right)\in G} o^+_{ij}$$

and let d_k denote the index of a vertex $v_k \in G$.

Proposition 2.3.1. *Let m be number of edges.Then*

$$E\left(G\right) \leq \sum_{k\in G} \sqrt{d_k} \leq \sqrt{2mn}$$

.

Proof. By *Theorem* 2.2.4, there is a maximal orthogonal symmetric matrix $O = [o_{ij}]$ such that $E\left(G\right) = \sum_{i\neq j, \left(i,j\right)\in G} o_{ij}$.Let

$$o^+ = \sum_{j, i\neq j, \left(i,j\right)\in G} o^+_{ij}$$

By Cauchy Schwarz inequality, $(o^+)^2 \leq d_i \sum_{j, i\neq j, \left(i,j\right)\in G} (o^+_{ij})^2 \leq d_i$. Hence $o^+ \leq \sqrt{d_i}$ and $E\left(G\right) \leq \sum_i o^+_i \leq \sum_i \sqrt{d_i}$. Since $\sum_k d_k = 2m$.
We get the inequality,

$$E\left(G\right) \leq \sqrt{2mn}$$

□

Let $E_n = max_{G\in S_n} E\left(G\right)$. We say that an orthogonal symmetric matrix $O = [o_{ij}]$ is extremal if $E_n = \sum_{i\neq j} o^+_{ij}$ and for $G \in S_n$ that it is an extremal energy graph if $E_n = E\left(G\right)$.

For a given real matrix $M = [m_{ij}]$, we define a graph $G = G_M$ by $(v_i, v_j) \in G$ if and only if $m_{ij} > 0$. Since $E\left(G, O\right) = \sum_{i\neq j, (i,j)\in G} o_{ij} \leq \sum_{i\neq j} o^+_{ij}$ and $E\left(G_O, O\right) = \sum_{i\neq j} o^+_{ij}$, by *Theorem* 2.2.4, we get:

Proposition 2.3.2. *For every integer $n \geq 1$,*

$$E_n = max_{O \in O^S(n)} \sum_{i \neq j} o_{ij}^+ = \frac{1}{2} max_{O \in O^S(n)} \big(\sum_{i \neq j} o_{ij} + |o_{ij}| \big)$$

and there is an orthogonal symmetric extremal matrix $O = [o_{ij}]$ and an extremal energy graph $G \in Sn$.

Since $O \in O^S(n)$ if and only if $-O \in O^S(n)$, we have $|\sum o_{ij}| \leq n$ for $O \in O^S(n)$

Proposition 2.3.3. *Suppose that a matrix $O = [o_{ij}]$ of type $n \times n$ is an orthogonal symmetric extremal matrix. Then $E_n = E_n^1 := \frac{1}{2} + \frac{3}{2} n^{\frac{3}{2}}$ if and only if*

(1) $\sum\limits_j o_{ij} = 1$

(2)$|o_{ij}| = 1/\sqrt{n}$

(3)$o_{ij} \leq 0$

Proof. Let $P = \big(I + O\big)/2$. If $E_n = E_n^1$, then $\sum o_{ij} = n$. Hence $|pv|^2 = n$ and therefore $Pv = v$; so we get (a). The condition (a) can be replaced with $\sum o_{ij} = n$. □

We can verify that $E_n = \frac{1}{2} + \frac{3}{2} n^{\frac{3}{2}}$ for $n = 4^k$ using orthogonal matrices. We construct orthogonal matrices $O_n, n = 4^k$, of type $n \times n$ with elements $o_{ij} = \pm 1/\sqrt{n}$ by induction (we first construct A_{4^k}):

$$A_3 = \begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}$$

We also need B_4:

$$B_3 = \begin{bmatrix} 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \end{bmatrix}$$

Using the tensor product we define $A_{4^{k+1}} = B_4 \otimes A_{4^k}$:

$$A_{4^{k+1}} = \begin{bmatrix} A_{4^k} & A_{4^k} & A_{4^k} & -A_{4^k} \\ A_{4^k} & A_{4^k} & -A_{4^k} & A_{4^k} \\ A_{4^k} & -A_{4^k} & A_{4^k} & A_{4^k} \\ -A_{4^k} & A_{4^k} & A_{4^k} & A_{4^k} \end{bmatrix}$$

Let $O_n = 1/\sqrt{n}A_n$. Using $Proposition$ 2.2.3, we can verify that the matrices On are extremal for $n = 4^k$.For $n = 4$ the complete graph is extremal, $E_4 = 2.3 = 6$; the matrix $O_4 = \frac{1}{2}A_4$ is extremal. For $n = 4^2 = 16$, the matrix $O_{16} = \frac{1}{4}B_4 \otimes A_4$ is extremal: $|O_{16}^+| = \sum\limits_{i \neq j} o_{ij}^+ = 12.12/4 + 44/4 = 36 + 4 = 40 = E_{16}$;
$|O_{16}|/2 = 16\sqrt{16}/2 = 32$

2.4 Hyperenergetic Graphs

The energy of a graph increases with the increase of the number of vertices and edges. Among n vertex graphs,the complete graph K_n has maximal energy. It was soon shown that there exist graphs whose energy exceeds $E\big(K_n\big)$ and $E\big(K_n\big) = 2n - 2$

Definition 2.4.1. *A graph G,such that* $E\big(K_n\big) > 2n - 2$ *is said to be hyperenergetic.*

Proposition 2.4.2. *Let G be* $\big(p, q\big)$ *graph with* $q \geq 2p$*.The line graph of the complete graph on n vertices is hyperenergetic if* $n \geq 5$*.*

Proof. The complete graph K_n is regular of degree $n-1$.The line graph of K_n has $n(n-1)/2$ vertices.Then the characterstic polynomial of a regular graph R and of its line graph $L(G)$ are related as

$$\phi(L(R),x) = (x+2)^{n(r-2)/2}\phi(R, x-r+2)$$

where n and r the number of vertices and degree of R.

Then

$$\phi(K_n,x) = (x-n+1)(x+1)^{n-1}.$$

we calculate,

$$E(L(K_n)) = 2n^2 - 6n$$

which for $n \geq 5$ is greater than

$$E(k_{n(n-1)/2}) = n^2 - n - 2.$$

□

Corollary 2.4.3. *It is possible to construct hyperenergetic graphs with n vertices for every $n \geq 9$.*

Proof. Let G be (p,q) graph with $q \geq 2p$.

Then $L(G)$ is hyperenergetic (n,m) graph'

Using Cauchy Schwarz Inequality,

$$\Big(\sum_{i=1}^{N} a_i b_i\Big)^2 \leq \sum_{i=1}^{N} a_i^2 \sum_{i=1}^{N} b_i^2$$

Choosing $N = p, a_i = \delta_i$ and $b_i = 1$.

Using (1.1) and (1.2) We arrive at

$$\begin{aligned} m &= \frac{1}{2}\sum_{i=1}^{p}\delta_i^2 - q \\ &\geq \frac{1}{2}\frac{\left(2q\right)^2}{p} - q \\ &\geq 3q \\ &= 3n \end{aligned}$$

Since $L\left(G\right)$ has more than $2n$ edges.By *proposition* 2.4.2 can be applied to it. □

Corollary 2.4.4. *Let $p \geq 5$, let G be a $\left(p,q\right)$ graph.If $q \geq 2p$, then $L^2\left(G\right)$ is hyperenergetic.*

Corollary 2.4.5. *Let $p \geq 5$, let G be a $\left(p,q\right)$ graph.If $q \geq 2p$ then all iterated line graphs $L^i\left(G\right), i = 2, 3, \ldots,$ are hyperenergetic.*

Chapter 3

Maximal Energy Graphs

If G is a graph on n vertices,then $E\big(G\big) \leq \frac{n}{2}\big(1+\sqrt{n}\big)$ must hold and that this bound is sharp if and only if G is strongly regular graph with parameters given by certain functions of n. Strongly regular graphs with these parameters have been called maximal energy graphs.This enables us to find an infinite family of maximal energy graphs.Using result on Hadamard difference sets,we construct regular graphical Hadamard matrices of negative type of order $4m^4$ for every integer m.If $m > 1$,such a Hadamard matrix is equivalent to a strongly regular graph with parameters $\big(4m^4, 2m^4+m^2, m^4+m^2, m^4+m^2\big)$.

3.1 Maximal Energy Graphs

Definition 3.1.1. *A strongly regular graph (srg) with parameters* $\big(n,k,\lambda,\mu\big)$ *is a graph with* n *vertices that is regular of valency* $k\big(1 \leq k \leq n-2\big)$ *and that has the following properties:*

○ *For any two adjacent vertices* x, y *there are exactly* λ *vertices adjacent to both* x *and* y*.*

○ *For any two non adjacent vertices* x, y *there are exactly* μ *vertices adjacent* *to both x and y.*

If $\mu = 0$, then G is a disjoint union of complete graphs, whereas, if $\mu \geq 1$ and G is non-complete, then the eigenvalues of G are k (the trivial eigenvalue) and the roots r, s of the quadratic equation

$$x^2 + \mu - \lambda x + \mu - k = 0 \tag{3.1}$$

The eigenvalue k has multiplicity one, whereas the multiplicities m_r of r and m_s of s can be calculated by solving the simultaneous equations

$$m_r + m_s = n - 1,\ k + m_r r + m_s s = 0$$

Theorem 3.1.2. *If $2m \geq n$ and G is a graph on n vertices with m edges, then the inequality*

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)[2m - (\frac{2m}{n})^2]} \tag{3.2}$$

holds. Moreover, equality holds if and only if G is either $\frac{n}{2}K_2, K_n$, or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\left(2m - (\frac{2m}{n})^2\right)/(n-1)}$.

Proof. Suppose that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ are the eigen values of G(which are real symmetric).Then we have

$$\lambda_1 \geq \frac{2m}{n}.$$

Moreover,since

$$\sum_{i=1}^{n} \lambda_i^2 = 2m$$

must hold.We have

$$\sum_{i=2}^{n} \lambda_i^2 = 2m - \lambda_1^2$$

Using this together with the Cauchy Schwarz inequality, applied to the vectors $\big(|\lambda_1|, |\lambda_2|, \ldots, |\lambda_n|\big)$ and $\big(1, 1, \ldots, 1\big)$ with $n-1$ entries, we obtain the inequality

$$\sum_{i=2}^{n} |\lambda_i| \leq \sqrt{(n-1)[2m - \lambda_1^2]}$$

Thus we must have

$$E\big(G\big) \leq \lambda_1 + \sqrt{(n-1)[2m - \lambda_1^2]}$$

Now the function $F(x) : x + \sqrt{(n-1)^2[2m - x^2]}$ decreases the interval $\sqrt{\frac{2m}{n}} < x \leq \sqrt{2m}$ in view of $2m \geq n$.

We see that $\sqrt{\frac{2m}{n}} \leq \frac{2m}{n} \leq \lambda_1$ must hold and hence $F\big(\lambda_1\big) \leq F\big(\frac{2m}{n}\big)$ must hold.

From this,

$$E\big(G\big) \leq \frac{2m}{n} + \sqrt{(n-1)[2m - (\frac{2m}{n})^2]} \quad \text{holds.}$$

As the eigen value for $\frac{n}{2}K_2$ are ± 1(both with multiplicity $\frac{n}{2}$) and the eigen values of K_n are $n-1$ and -1.

That is G is one of the graphs given in the second part of the theorem, then equality must hold in (3.2).

Conversely, if equality holds in (3.2), then by the previous discussion on the function $F(x)$ we see that $\lambda_1 = \frac{2m}{n}$ must hold.

Therefore it follows that G is regular with valence $\frac{2m}{n}$. Now, since equality must also hold in the Cauchy Schwarz inequality given above, we have

$$|\lambda_i| \leq \sqrt{\big(2m - (\frac{2m}{n})^2\big)/(n-1)}, \text{for } 2 \leq i \leq n$$

Hence, we are reduced to three possibilities:

1) either G has two eigenvalues with equal absolute values, in which case G must equal $\frac{n}{2}K_2$.

2) G has two eigenvalues with distinct absolute values, in which case G must equal K_n.

3) G has three eigenvalues with distinct absolute values equal to $\frac{2m}{n}$ or $\sqrt{\left(2m - \left(\frac{2m}{n}\right)^2\right)/(n-1)}$, in which case G must be a non-complete connected strongly regular graph as required. $\square$

Theorem 3.1.3. *If $2m \leq n$ and G is a graph on n vertices with m edges, then the inequality*

$$E\big(G\big) \leq 2m$$

holds. Moreover, equality holds if and only if G is disjoint union of edges and isolated vertices.

Proof. Since $2m \leq n$, it follows that G must have atleast $n - 2m$ isolated vertices.

Consider the graph G' that is obtained from G by removing $n - 2m$ isolated vertices. Then G' has $2m$ vertices and m edges.

Thus we may apply $Theorem$ 3.1.2 to immediately see that $E\big(G'\big) \leq 2m$ must hold, with equality holding if and only if G' is the disjoint union of edges. The proof of the theorem now immediately follows. $\square$

Theorem 3.1.4. *Let G be a graph of n vertices.Then*

$$E\big(G\big) \leq \frac{n}{2}(1 + \sqrt{n})$$

holds with equality holding if and only if G is strongly regular graph with parameters $\big(n, \big(n + \sqrt{n}\big)/2, \big(n + 2\sqrt{n}\big)/4, \big(n + \sqrt{n}\big)/4\big)$.

Proof. Suppose G be a graph of n vertices and m edges.

If $2m \geq n$,then the equality

$$E \leq \frac{2m}{n} + \sqrt{(n-1)[2m - \frac{2m}{n}^2]}$$

and is considered as a function of m is maximized when $m = \frac{n^2+n\sqrt{n}}{4}$ substitute the value of m to (3.2) we get

$$E(G) \leq \frac{n}{2}(1+\sqrt{n})$$

Moreover,it follows by $Theorem$ 3.1.2 and (3.1) that equality holds in $E(G) \leq \frac{2m}{n} + \sqrt{(n-1)[2m - \frac{2m}{n}^2]}$ if and only if G is a strongly regular graph with parameters $(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+\sqrt{n})/4)$.

If $2m \leq n$, then by $Theorem$ 3.1.4, $E(G) \leq n$

Therefore the proof of the theorem follows immediately. □

We note that an strongly regular graph with the parameters $(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+2\sqrt{n})/4)$ will be called a **maximal energy** of order n. The compliment of a maximal energy graph is a strongly regular graph with parameters $(n, (n-\sqrt{n})/2, (n-2\sqrt{n})/4, (n-2\sqrt{n})/4)$. However the strong regular graph doesnot have maximal energy.Consider a family of maximal energy graph pf order 4^k, maximal energy graph of order n exist for all even squares.To support this conjecture the case $n = 4m^4$with m even.In this chapter we show maximal energy graph of order $4m^4$ also exist for all odd integers.

Theorem 3.1.5. *A maximal energy graph of order* $4m^4$ *exists for every positive integer* m

3.2 Regular Graphical Hadamard Matrix

A Hadamard matrix of order n is $n \times n$ matrix H with entries ± 1 such that

$$HH^T = nI_n, \text{where } I_n \text{ is the identity matrix of order } n.$$

we will see below that maximum energy graphs are essentially the same objects as certain special Hadamard matrix.

Definition 3.2.1. *A Hadamard matrix is said to be graphical if it is symmetric and it has constant diagonal.*

Note that if H is a graphical Hadamard matrix of order n with δ on the diagonal and J is the $n \times n$ all ones matrix then $A = \frac{1}{2}\big(J - \delta H\big)$is the adjacency ,matrix of a graph of n vertices.

Definition 3.2.2. *A Hadamard matrix is said to be regular if all its row and column sums are constant.*

Let H be a Hadamard matrix of order n. If H is regular, then there exists an integer l such that $H\mathbf{1} = H^T\mathbf{1} = l\mathbf{1}$. Since $HH^T = nI_n$, we have $l^2\mathbf{1} = n\mathbf{1}$. Hence $l = \pm\sqrt{n}$.

Definition 3.2.3. *Let H be a regular graphical Hadamard matrix with row sum l and δ on the diagonal. We say that H is of positive type, or type $+1$ (respectively, negative type, or type -1) if $\delta l > 0$ (respectively, $\delta l < 0$).*

It has been observed that if H is a regular graphical Hadamard matrix with δ on its diagonal, of type ε,then $A = \frac{1}{2}\big(J - \delta H\big)$ is the adjacency matrix of an strongly regular graph with parameters

$$\big(n, \big(n - \varepsilon\sqrt{n}\big)/2, \big(n - 2\varepsilon\sqrt{n}\big)/4, \big(n - 2\varepsilon\sqrt{n}\big)/4\big).$$

Conversely, if A is the adjacency matrix of an strongly regular graph with this parameters then $J - 2A$ is a regular graphical Hadamard matrix of type ε. Thus a maximum energy graph is essentially the same as a regular graphical Hadamard matrix of negative type.

Lemma 3.2.4. *If there exist a regular graphical Hadamard matrix of order* n *of positive, or negative type, then there exist regular graphical Hadamard matrices of order* $4n$ *of both types.*

In particular, we can make regular graphical Hadamard matrices of order 4^k of any type for all positive integers k. Hence, for n a power of 4, there exist strongly regular graphs with parameters for $\varepsilon = 1$ and for $\varepsilon = -1$. So we can conclude that maximal energy graphs exist for all orders $n = 4k$.

Theorem 3.2.5. *For every positive integer* m *there exists a regular graphical Hadamard matrix of order* $4m^4$ *of positive, as well as of negative type.*

In the Seidel Switching Section, we show how in this case the negative type can be obtained from the positive type(and vice versa).

Definition 3.2.6. *Let* G *be a finite group of order* n*. A* k*-element subset* D *of* G *is called a* (n, k, λ) *difference set in* G *if the list of "differences"* $d_1 d_2^{-1}$, $d_1, d_2 \in D, d_1 \neq d_2$*, represents each non-identity element in* G *exactly* λ *times. Using multiplicative notation for the group operation,* D *is a* (n, k, λ) *difference set in* G *if and only if it satisfies the following equation in* $Z[G]$*:*

$$DD^{(-1)} = (K - \lambda)1_G + \lambda G$$

where $D = \sum_{d \in D} d$, $D^{(-1)} = \sum_{d \in D} d^{(-1)}$ *and* 1_G *is the identity element of* G*.A subset* D *of* G *is called reversible if* $D^{(-1)} = D$*. The difference sets considered in this note have parameters*

$$(n, k, \lambda) = (4n^2, 2n^2 \pm n, n^2 \pm n)$$

These difference sets are called Hadamard difference sets, since their $(1, -1)$*-incidence matrices are Hadamard matrices.*

Lemma 3.2.7. *Let t be a positive integer and let D be a reversible $(4t^2, 2t^2+t, t^2+t)$ Hadamard difference set in a group G of order $4t^2$ such that $1_G \neq D$. Then there exists a $4t^2 \times 4t^2$ regular graphical Hadamard matrix of negative type.*

Proof. Let $Cay(G, D)$ be the Cayley graph with vertex set G and connection set D. That is, the vertex set of $Cay(G, D)$ is G, two vertices $x, y \in G$ are connected by an edge if and only if $xy^{-1} \in D$. Let A be the adjacency matrix of $Cay(G, D)$. Since $1_G \neq D$, the diagonal entries of A are all zeros. Also A is symmetric because D is reversible. Since D is a Hadamard difference set, we have

$$A^2 = t^2 I + (t^2 + t)J$$

Now let $H = J - 2A$. Then H is symmetric.Since A is the diagonal entries of H are all ones ($i.e., \delta = 1$). The row sums of H are constant, and they are equal to $l = 4t^2 - 2(2t^2 - 1) = -2t$. Hence

$$\delta l = -2t < 0$$

Furthermore, from $A^2 = t^2 I + (t^2 + t)J$, we have

$$H^2 = 4t^2 I$$

Therefore,H is regular graphical Hadamard matrix of negative type. □

Theorem 3.2.8. *Let $K = \{1, a, b, ab\}$ be a klein four group.Let*

$$E_1 = (1, A_0) \cup (a, A_1) \cup (b, A_2) \cup (ab, A_3)$$

and

$$E_2 = (1, B_0) \cup (a, B_1) \cup (b, B_2) \cup (ab, B_3)$$

be reversible Hadamard difference sets in groups $K \times W_1$ *and* $K \times W_2$ *respectively, where* $|W_1| = w_1^2$ *and* $|W_2| = w_2^2$, w_1 *and* w_2 *are odd* $A_i \subseteq W_1$ *and* $B_i \subseteq W_2$ *and*

$$|A_0| = |A_1| = |A_2| = \frac{w_1^2 - w_1}{2}$$

$$|B_0| = |B_1| = |B_2| = \frac{w_2^2 - w_2}{2}$$

$$|A_3| = \frac{w_1^2 + w_1}{2}$$

$$|B_3| = \frac{w_2^2 + w_2}{2}$$

Let $E = \big(1, \bigtriangledown(A_0, A_1 : B_0, B_1)\big) \cup \big(a, \bigtriangledown(A_0, A_1 : B_2, B_3)\big)$
$\cup \big(b, \bigtriangledown(A_2, A_3 : B_0, B_1)\big) \cup \big(ab, \bigtriangledown(A_2, A_3 : B_2, B_3)\big)$
Then

$$|\bigtriangledown(A_0, A_1 : B_0, B_1)| = |\bigtriangledown(A_0, A_1 : B_2, B_3)| = |\bigtriangledown(A_2, A_3 : B_0, B_1)| = \frac{w_1^2 w_2^2 - w_1 w_2}{2}$$

$$| \bigtriangledown (A_2, A_3 : B_2, B_3)| = \frac{w_1^2 w_2^2 + w_1 w_2}{2}$$

and E *is reversible* $\big(4w_1^2 w_2^2,\ 2w_1^2 w_2^2 - w_1 w_2,\ w_1^2 w_2^2 - w_1 w_2\big)$ *Hadamard difference set in the group* $K \times W_1 \times W_2$.

Proposition 3.2.9. *Let* $m > 1$ *be an integer and* $m = p_1 p_2 \dots p_t$*,where* $p_i, i = 1, 2, \dots t$ *are (not necessarily distinct) odd primes.Let* $K = \{1, a, b, ab\}$ *be a klein four group and* $W = Z_{P_1}^4 \times \dots \times Z_{P_i}^4$*.Then there exist a reversible Hadamard difference set* E *in* $G = K \times W$ *such that*

$$E_1 = (1, E_0) \cup (a, E_1) \cup (b, E_2) \cup (ab, E_3)$$

where $E_1 \subset W$,$|E_0| = |E_1| = |E_2| = \frac{m^4-m^2}{2}, |E_3| = \frac{m^4+m^2}{2}$ *and* $1_w \neq E_i$ *for* $i = 0, 1, 2$ *but* $1_w \in E_3$.

Proof. We use induction on t.

If $t = 1$,the the construction following the proof of $Lemma$ 3.2.7 and preceding $Theorem$ 3.2.8 guarantees the existence of the required difference set.

Assume that the proposition is true when m is a product of $(t-1)$ primes.

We will prove that the proposition is true when $m = p_1p_2 \dots p_t$, where $p_i, i = 1, 2, \dots, t$ are odd primes.

Let $w_1 = p_1^2p_2^2 \dots p_{t-1}^2$.

Then by induction hypothesis, there exists a reversible difference set

$$E_1 = (1, A_0) \cup (a, A_1) \cup (b, A_2) \cup (ab, A_3)$$

in $K \times W_1$

where $W_1 = Z_{P_1}^4 \times \dots \times Z_{P_i}^4$,$A_i \subset W_1$ for all $i = 0, 1, 2, 3$

$$|A_0| = |A_1| = |A_2| = \frac{w_1^2 - w_1}{2}$$

$$|A_3| = \frac{w_1^2 + w_1}{2}$$

and $1_{w_1} \neq A_i$ for $i = 0, 1, 2$ but $1_{w_1} \in A_3$

Let $w_2 = p_t^2$.Again by the proof $Lemma$ 3.2.7,there a reversible difference set

$$E_2 = (1, B_0) \cup (a, B_1) \cup (b, B_2) \cup (ab, B_3)$$

in $K \times W_2$,

where $W_2 = Z_{p_t}^4$, $B_i \subset W_2$ for all $i = 0, 1, 2, 3$

$$|B_0| = |B_1| = |B_2| = \frac{w_2^2 - w_2}{2}$$

$$|B_3| = \frac{w_2^2 + w_2}{2}$$

and $1_{w_2} \neq B_i$ for $i = 0, 1, 2$ but $1_{w_2} \in B_3$

Then by *Theorem* 3.2.8

$$E = \big(1, \triangledown(A_0, A_1 : B_0, B_1)\big) \cup \big(a, \triangledown(A_0, A_1 : B_2, B_3)\big)$$

$$\cup\big(b, \triangledown(A_2, A_3 : B_0, B_1)\big) \cup \big(ab, \triangledown(A_2, A_3 : B_2, B_3)\big)$$

is a reversible Hadamard difference set in $K \times W_1 \times W_2 = K \times W$ and

$$|\triangledown(A_0, A_1 : B_0, B_1)| = |\triangledown(A_0, A_1 : B_2, B_3)| = |\triangledown(A_2, A_3 : B_0, B_1)| = \frac{m^4 - m^2}{2}$$

$$| \triangledown (A_2, A_3 : B_2, B_3)| = \frac{m^4 + m^2}{2}.$$

Next it is straight forward that

$1_w \neq \triangledown(A_0, A_1 : B_0, B_1)$,

$1_w \neq \triangledown(A_0, A_1 : B_2, B_3)$,

$1_w \neq \triangledown(A_2, A_3 : B_0, B_1)$ but $1_w \in \triangledown(A_2, A_3 : B_2, B_3)$.

Hence the proof. □

Theorem 3.2.10. *Let m be a positive odd integer.Then there exist $4m^4 \times 4m^4$ regular graphical Hadamard matrix of negative type.*

Proof. When $m = 1$, one can easily demonstrate a 4×4 regular graphical Hadamard matrix of negative type. Therefore we will assume that m is an odd integer greater than 1.

By *propostion* 3.2.9 there exist a reversible Hadamard difference set

$$E_1 = (1, E_0) \cup (a, E_1) \cup (b, E_2) \cup (ab, E_3)$$

in a group $G = K \times H$ where $K = \{1, a, b, ab\}$ be a klein four group and H is an abelian group of order m^4 such that

$$|E_0| = |E_1| = |E_2| = \frac{m^4 - m^2}{2}, |E_3| = \frac{m^4 + m^2}{2}$$

and $1_H \neq E_i$ for $i = 0, 1, 2$ but $1_H \in E_3$.

Let $E' = \big(K \times H\big)/E$.That is E' is compliment of E,and let $D = \big(ab, 1_H\big)E'$.Then D is a reversible $(4m^4, 2m^4 + m^2, m^4 + m^2)$ Hadamard difference set in $K \times H$ since

$$D = (ab, E_0') \cup (b, E_1') \cup (a, E_2') \cup (1, E_3')$$

and $1_H \neq E_3'$.We see that $1_G \neq D$.

Apply *Lemma* 3.2.7(with $t = m^2$),

we conclude that there exist $4m^4 \times 4m^4$ regular graphical Hadamard matrix of negative type. □

3.3 Seidel Switching

Consider a graphical Hadamard matrix H of order n. Let X be a subset of $\{1, \ldots, n\}$. If we multiply rows and columns indexed by X by -1, we again obtain a graphical Hadamard matrix. The operation on the corresponding graph is called Seidel switching. In some cases it is possible to switch a graphical Hadamard matrix of positive type into one of negative type (and vice versa). Here we will show that this is indeed the case for the graphical Hadamard matrices constructed, which leads to graphical Hadamard matrices of negative type constructed in the previous section.

Lemma 3.3.1. *Suppose*

$$H = \begin{bmatrix} H_1 & H_{12} \\ -H_{12}^T & H_2 \end{bmatrix}$$

is a regular graphical Hadamard matrix of order n. Furthermore assume that H_1

and H_2 have row sum 0. Then there exist regular graphical Hadamard matrix of order n of positive type, as well as one of negative type.

Proof. Consider

$$H' = \begin{bmatrix} H_1 & -H_{12} \\ -H_{12}^T & H_2 \end{bmatrix}$$

Then H' clearly is again a graphical Hadamard matrix with the same diagonal as H.

Let l be the row sum of H.

Then, since H_1 and H_2 have row sum 0, H_12 has row and column sum l. This implies that H' is regular with row and column sum $-l$. So the type of H' is opposite to the type of H. □

3.4 Bounds for the energy

Theorem 3.4.1. *If G is a graph with n vertices, m edges and adjacency matrix A,then*

$$\sqrt{2m + n(n-1)|detA|^{\frac{2}{n}}} \leq E\big(G\big) \leq \sqrt{2mn}.$$

Proof. We have

$$\sum_{j=1}^{n} \lambda_j^2 = 2m$$

and start with

$$\begin{aligned}\big[E\big(G\big)\big]^2 &= \left(\sum_{j=1}^{n} |\lambda_j|^2\right) \\ &= \sum_{j=1}^{n} |\lambda_j|^2 + 2\sum_{j<k} |\lambda_j||\lambda_k| \qquad (3.3) \\ &= 2m + n(n-1)AM\{|\lambda_j||\lambda_k|\}\end{aligned}$$

where $AM\{|\lambda_j||\lambda_k|\}$ indicates the arithemetic mean of the $\frac{n^2-n}{2}$ distinct terms $|\lambda_j||\lambda_k|, j < k$.

The geometric mean of the same term is

$$\begin{aligned} GM\{|\lambda_j||\lambda_k|\} &= \left(\prod_{j<k} |\lambda_j||\lambda_k|\right)^{\frac{2}{n^2-n}} \\ &= \left(\prod_{j=1}^{n} |\lambda_j|^{n-1}\right)^{\frac{2}{n^2-n}} \\ &= \left(\prod_{j=1}^{n} |\lambda_j|^{n-1}\right)^{\frac{2}{n}} \\ &= |detA|^{\frac{2}{n}} \end{aligned}$$

where we have taken into account that $\prod_{j=1}^{n} \lambda_j = detA$.

The lower bound is now a consequence of the fact that the geometric mean of non negative numbers cannot exceed their arithmetic mean.

The variance of the numbers $|x_j|, j = 1, 2, \ldots, n$

$$\begin{aligned} var\{|\lambda_j|\} &= AM\{|\lambda_j|^2\} - [AM\{|\lambda_j|\}]^2 \\ &= \frac{1}{n}\sum_{j=1}^{n} |\lambda_j|^2 - \left[\frac{1}{n}\sum_{j=1}^{n} |\lambda_j|\right]^2 \\ &= \frac{2m}{n} - \frac{E^2}{n^2} \\ &= \frac{2m}{n} - \left(\frac{E}{n}\right)^2 \end{aligned}$$

and the upper bound follows from the fact that the variance is a non negative quantity. □

Corollary 3.4.2. *If $detA \neq 0$, then $E(G) \geq \sqrt{2m + n(n-1)} \geq n$.*

Also the relation

$$\sum_{j<k} \lambda_j \lambda_k = -m.$$

Then (3.3) becomes,

$$E^2 = 2m + \sum_{j<k} |\lambda_j||\lambda_k|$$
$$\geq 2m + 2|\sum_{j<k} \lambda_j \lambda_k|$$
$$= 2m + 2|-m|$$
$$= 4m$$
$$ie, E \geq 2\sqrt{m}.$$

If G has isolated vertices,then each isolated vertices results in an eigen value equal to zero.

Adding isolated vertices of G will thus change neither m nor E.Consider for a moment, graphs having m edges and no isolated vertices.The maximum number of vertices of such graphs $2m$,which happens if $G = mK_2$.ie,if the graph G consist of m isolated edges.

For all other graphs $n < 2m$,we have

$$\sqrt{2mn} \leq \sqrt{2m(2m)} = 2m,$$

which is combined with the upper bound

$$E \leq 2M.$$

Corollary 3.4.3. *If G is a graph containing m edges, then*

$$2\sqrt{m} \geq E \leq 2m. \tag{3.4}$$

The bound is sharp: $E\big(G\big) = 2\sqrt{m}$ holds if and only if G is complete bipartite graph plus arbitrarily many isolated vertices and $E\big(G\big) = 2m$ hold if and only if G consists of m isolated edges and of arbitrarily ,any isolated vertices. Thus among lower and upper bounds for E ,depending solely of m.

In some cases the lower bound can be improved.That is we have that the greatest eigen value of a graph cannot be less than the average vertex degree $\frac{2m}{n}$

$$\frac{2m}{n} \leq \lambda_1 \leq \sum_{+} \lambda_j = \frac{1}{2}E$$

$$ie, E \geq \frac{4m}{n} \tag{3.5}$$

This estimate is better than the lower bound in (3.4) if

$$\frac{n^2}{4} < m \leq \frac{n(n-1)}{2}.$$

Equality (3.5) occurs if and only if G is a complete multipartite graph.

CONCLUSION

In this dissertation we discuss the maximal energy graphs.Here we provide the method to improve the upper bound for the energy.Energy of the graph is solely depends on the vertices and edges of the graph.By doing the project we came to know more about the energy of different graphs with matrix such as orthogonal matrix.And resulting the graph having maximal energy when they are strongly regular graph with certain parameters holds.They are equivalent to certain hadamard matrices.

Bibliography

[1] I.Gutman:The Energy of Graph:old and new results.Springer,Berlin(2001).

[2] J.H.Koolen,V.Moulten: Maximal energy graphs.Adv.Appl.Math 26(2001).

[3] Walter Gautschi,Giuseppe Mastroianni,Themistocles M.Rassias(Editors): Approximation and Computation, Springer(2011).

[4] W.H.Haemers: Strongly regular graphs with maximal energy,Linear algebra Appl.429(2008).

[5] Xueliang L.,Yongtang Shi,Ivan Gutman: Graph Energy, Springer(2012).