ENERGY OF GRAPHS AND DIGRAPHS

NAFISEH JAHANBAKHT
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This thesis is dedicated to Dr. Kourosh Tavakoli.

Abstract

The energy of a graph is the sum of the absolute values of the eigenvalues of its adjacency matrix. The concept is related to the energy of a class of molecules in chemistry and was first brought to mathematics by Gutman in 1978 ([8]). In this thesis, we do a comprehensive study on the energy of graphs and digraphs.

In Chapter 3, we review some existing upper and lower bounds for the energy of a graph. We come up with some new results in this chapter. A graph with n vertices is hyper-energetic if its energy is greater than $2n-2$. Some classes of graphs are proved to be hyper-energetic. We find a new class of hyper-energetic graphs which is introduced and proved to be hyper-energetic in Section 3.3.

The energy of a digraph is the sum of the absolute values of the real part of the eigenvalues of its adjacency matrix. In Chapter 4, we study the energy of digraphs in a way that Peña and Rada in [19] have defined. Some known upper and lower bounds for the energy of digraphs are reviewed. In Section 4.5, we bring examples of some classes of digraphs in which we find their energy.

Keywords. Energy of a graph, hyper-energetic graph, energy of a digraph.

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Chapter 1

Introduction

The concept of the energy of a graph was introduced three decades ago by Ivan Gutman [8]. This notion is related to the total electron energy of a class of organic molecules in computational chemistry. The total energy of the so-called π-electrons is calculated by the formula

$$\mathcal{E}_\pi = \sum_{j=1}^{n} |\lambda_j| \tag{1.1}$$

where n is the number of the molecular orbital energy levels and λ_js are eigenvalues of the adjacency matrix of the so-called molecular or Hückel graph. Although in chemistry the expression (1.1) is valid only for the class of "Hückel graphs", the right-hand side of (1.1) is well-defined for any class of graphs in mathematics. This motivated Gutman to define the energy of a graph.

Definition 1.0.1 [8] Let G be a graph, the *energy* of G, denoted by $\mathcal{E}(G)$, is the sum of the absolute values of the eigenvalues of G, i.e. if $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of G, then $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$.

For one example, by using the eigenvalues found in page 14, the energy of a complete graph of order n is computed as

$$\mathcal{E}(K_n) = |n-1| + |-1|(n-1) = 2n-2 \ .$$

There are some bounds on the energy of a graph. In this thesis, we mention some of the most well-known bounds. For a graph G of order n with m edges, McClelland ([17]) in early 70's, gave the following general bounds on its energy where A is the adjacency matrix of G.

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

A lower bound for the energy of a graph only in terms of its number of edges is $\mathcal{E}(G) \geq 2\sqrt{m}$ with equality if and only if G is a complete bipartite graph plus some isolated vertices. In terms of the number of vertices the lower bound is $\mathcal{E}(G) \geq 2\sqrt{n-1}$ with equality if and only G is the star $K_{1,n-1}$.

For the upper bound, there is a well-known result due to Koolen and Moulton ([14]) which is an improvement on the McCelland bound. For a graph G with n vertices and m edges where $2m \geq n$, they proved

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

with equality if and only if G is K_n, $\frac{n}{2}K_2$, or a strongly regular graph (SRG) with two eigenvalues having absolute value $\sqrt{\frac{(2m-(2m/n)^2)}{(n-1)}}$.

Next, if we consider the left hand side of the above inequality as a function of m, it is maximized when $m = (n^2 + n\sqrt{n})/4$. By substituting this amount in the above formula we find

$$\mathcal{E}(G) \leq \frac{n(1+\sqrt{n})}{2} \ . \tag{1.2}$$

Koolen and Moulton ([14]) proved that (1.2) is also valid for $2m < n$ and that the equality holds if and only if G is an SRG with parameters $(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+2\sqrt{n})/4)$.

They also conjectured that for a given $\varepsilon > 0$ there exists a graph G of order n such that for almost all $n \geq 1$, $\mathcal{E}(G) \geq (1-\varepsilon)\frac{n}{2}(\sqrt{n}+1)$ which was later proved in [18] by Nikiforov.

There was a conjecture in 1978 that between graphs of order n, the complete graph K_n has the maximum energy. Although it was rejected and it was shown that there exist subgraphs of K_n with energy greater than that of K_n, it was an introduction for defining hyper-energetic graphs. A graph G with n vertices is *hyper-energetic* if $\mathcal{E}(G) > 2n-2$. Some classes of graphs have shown to be hyper-energetic.

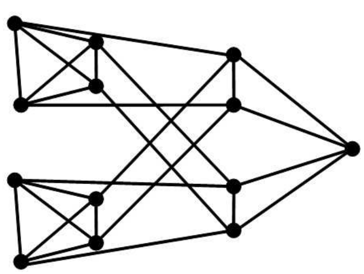


Figure 1.1: G_2

In this thesis, we introduce a new class of graphs which we prove that they are hyper-energetic. Our first example in this class is a 4-regular graph with 13 vertices that we call G_2 (see Figure 1.1).

In general case, we construct G_m as follows. Consider $2m-2$ copies of K_{2m} and m copies of K_2 and one copy of K_1. Add edges to make it $2m$-regular by adding $2m$ edges from the single vertex K_1 to vertices of m copies of K_2. Then add one edge from each vertex of K_{2m} to the m copies of K_2 (see Figure 3.4 in Section 3.3.1).

G_m is a $2m$-regular graph with $n = (2m-1)2m+1$ vertices. We found that the characteristic polynomial of G_m is $(x-2m)(x-(2m-1))^{2m-3}$ $(x+1)^{(2m-3)(2m-1)}(x^2-(2m-1))^m(x^2+2x-(2m-3))^m$ and from that we can find the energy of G_m. Then we prove that for $m > 2$, graph G_m is hyper-energetic.

If we want to generalize the concept of energy for the case of digraphs, we should be reminded that the adjacency matrix is not symmetric and the eigenvalues might be complex numbers. Peña and Rada in [19] proposed the following definition for the energy of digraphs.

Definition 1.0.2 Let $\mathcal{G}$ be a digraph, the energy of $\mathcal{G}$, denoted by $\mathcal{E}(\mathcal{G})$, is the sum of the absolute values of the real part of the eigenvalues of $\mathcal{G}$.

In fact, Peña and Rada proved the Coulson integral formula for the case of digraphs ([19]) and that was the motivation for the Definition 1.0.2.

As an example, consider the digraph $\mathcal{C}_4$ in Figure 1.2.

The characteristic polynomial of $\mathcal{C}_4$ equals x^4-1 and its eigenvalues are $1, -1, i, -i$. Therefore, $\mathcal{E}(\mathcal{C}_4) = 2$.

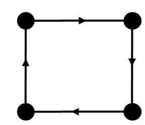


Figure 1.2: $\mathcal{C}_4$

Rada later in [20] and [21] found some lower and upper bounds for the energy of digraphs. The upper bound $\mathcal{E}(\mathcal{G}) \leq \sqrt{\frac{1}{2}n(m+c_2)}$ was found in [21] where n, m, and c_2 are number of vertices, number of arcs, and number of closed walks of length 2 respectively. The equality holds if and only if $\mathcal{G}$ is a digraph with $\dfrac{n}{2}$ copies of directed cycle of length 2. An upper bound solely in terms of the number of arcs of a digraph is $\mathcal{E}(\mathcal{G}) \leq m$ with equality if and only if $\mathcal{G}$ consists of $\frac{m}{2}$ copies of directed cycle of length 2 plus some isolated vertices.

The minimum energy for digraphs is 0 which is attained in acyclic digraphs. For the minimal energy of digraphs, Rada ([20]) found $\mathcal{E}(\mathcal{G}) \geq \sqrt{2c_2}$ where c_2 is the number of closed walks of digraph $\mathcal{G}$. The equality holds for acyclic digraphs or digraphs with exactly three eigenvalues $0, -\sqrt{c_2/2}, \sqrt{c_2/2}$ with multiplicities $n-2, 1, 1$ respectively.

Energy of digraphs is a new idea and not much work has been done on it. Energy of most classes of digraphs are not known. The results in this area are limited to the papers [19], [20], [21] of Peña and Rada. In this thesis, we focus on two classes of digraphs and we find their energy.

Let q be a prime power. Consider the finite field $\mathbb{F}_q$. Let S_q be the set of square elements of $\mathbb{F}_q$. Let $q \equiv 3 \pmod 4$. The Paley digraph is a directed graph $\mathcal{P}_q := (\mathcal{V}, A_q)$ with vertices $\mathcal{V} = \mathbb{F}_q$ and arcs $A_q =$

$\{(a,b)\in\mathbb{F}_q\times\mathbb{F}_q\ :\ b-a\in S\}$. In Section 4.5 we prove that the energy of Paley digraph $\mathcal{P}_q$ is one half of the energy of its underlying graph, K_q.

Let $H=[\mathbf{c}_1\ \mathbf{c}_2\ \ldots\ \mathbf{c}_n]$ be a Hadamard matrix of order $n=4m$ where $\mathbf{c}_i$s are columns of H and the last column equals all-one column. Define $C_i=\mathbf{c}_i\mathbf{c}_i^t$, $i=1,\cdots,n-1$. Consider a symmetric Latin square L of order n with numbers $\{1,\cdots,n\}$ and n on the diagonal ([13]). Construct the matrix M by changing each number i above the diagonal of L with C_i and each i below the diagonal of L with $-C_i$ and change the n on the diagonal with a $\mathbf{0}_{n\times n}$ matrix. Let D_1 be the matrix derived from M by changing 1 to 0 and -1 to 1, and D_2 be the matrix derived from M by changing -1 to 0. Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be their corresponding digraphs, respectively. The energy of the digraphs $\mathcal{G}_1$ and $\mathcal{G}_2$ is one half of the energy of their underlying graph as it is proved in Section 4.5.

Throughout, if we give a different proof of any result, we mention it.

# of vertices	# of edges	lower bound	equality occurs
n	m	$\sqrt{2m+n(n-1)\|det(A)\|^{\frac{2}{n}}}$	–
–	m	$2\sqrt{m}$	complete bipartite graph plus some isolated vertices
n	–	$2\sqrt{n-1}$	$K_{1,n-1}$
n	–	$\frac{n}{2}(\sqrt{n}-n^{1/10})$ for n sufficiently large	–

Table 1.1: Comparing lower bounds for the energy of graphs

# of vertices	# of edges	upper bound	equality occurs
n	m	$\sqrt{2mn}$	–
n	m $2m \geq n$	$\frac{2m}{n}+\sqrt{(n-1)(2m-(\frac{2m}{n})^2)}$	SRG with 2 eigenvalues $\|\lambda_1\| = \|\lambda_2\| = \sqrt{\frac{(2m-(2m/n)^2)}{(n-1)}}$
n	–	$\dfrac{n(1+\sqrt{n})}{2}$	SRG with parameters $(n, \frac{n+\sqrt{n}}{2}, \frac{n+2\sqrt{n}}{4}, \frac{n+2\sqrt{n}}{4})$

Table 1.2: Comparing upper bounds for the energy of graphs

# of vertices	# of edges	lower bound	upper bound	equality occurs
–	–	$\sqrt{2c_2}$	–	acyclic digraphs or digraphs with 3 eigenvalues 0, $\pm\sqrt{c_2/2}$
n	m	–	$\sqrt{\frac{1}{2}n(m+c_2)}$	$\frac{n}{2}$ copies of directed cycle of length 2
–	m	–	m	$\frac{m}{2}$ copies of directed cycle of length 2 +isolated vertices

Table 1.3: Comparing bounds for the energy of digraphs

Chapter 2

Preliminaries

In this section, we provide some basic definitions and useful propositions which are used throughout the thesis. The definitions are standard and are taken mostly from [7].

2.1 Basic Definitions

Throughout this thesis, we refer to a *graph* G (*digraph* $\mathcal{G}$) as an ordered pair $G := (V,E)$ ($\mathcal{G} := (V,A)$) where $V(G)$ ($V(\mathcal{G})$) is a set whose elements are called vertices, and $E(G)$ ($A(\mathcal{G})$) is a set of unordered (ordered) pairs of distinct vertices, called edges (arcs). We call a graph G (digraph $\mathcal{G}$) of order n if V is a set of n elements. The *underlying graph* of a diagraph is the graph obtained by replacing each arc of diagraph, i.e. ordered pairs, by corresponding undirected edge, i.e. unordered pairs.

The *adjacency matrix* of a graph G (*digraph* $\mathcal{G}$) of order n is the $n \times n$ $(0,1)$-matrix $A(G) = [a_{ij}]$ ($A(\mathcal{G}) = [a_{ij}]$), where $a_{ij} = 1$ if there is an edge (arc) connecting vertex i to vertex j, and $a_{ij} = 0$ otherwise.

A digraph $\mathcal{G}$ is *symmetric* if whenever $(v_i, v_j) \in A(\mathcal{G})$, then $(v_j, v_i) \in A(\mathcal{G})$. A one-to-one correspondence between graphs and symmetric digraphs is given by $\psi : G \rightarrow \check{G}$ where $\check{G}$ has the same vertex set as the graph G, and each edge $\{v_i, v_j\}$ of G is replaced by a pair of symmetric arcs (v_i, v_j) and (v_j, v_i). Under the correspondence ψ, a graph can be identified with a symmetric digraph.

The *degree* (*in-degree*) of a vertex v_i, denoted by d_i (d_i^-), is the number of edges ending at v_i. In a digraph, the *out-degree* of a vertex v_i, denoted by d_i^+, is the number of edges starting at v_i. The *degree sequence* of G is the non-increasing sequence of its vertex degrees. A graph of order n with an edge between any two vertices is a *complete graph*, denoted by K_n. A graph with no edges is called an *empty graph*. A *bipartite graph* is a graph whose vertices can be partitioned into two disjoint sets or parts so that the vertices within the same part are nonadjacent. A *complete bipartite graph* of order $m+n$, $K_{m,n}$, is a bipartite graph such that every pair of vertices in the two disjoint sets V_1 (with m vertices) and V_2 (with n vertices) are adjacent. The graph $K_{1,n-1}$ is called the *star graph*, denoted by S_n. A graph is *multipartite* if the set of vertices in the graph can be divided into non-empty subsets or parts, such that no two vertices in the same part have an edge connecting them. A *complete multipartite* graph is a multipartite graph such that any two vertices that are not in the same part have an edge connecting them.

The *complement* of a graph $G = (V, E)$ is a graph $\overline{G} = (V, \overline{E})$ where $\overline{E}$ is the complement of E with respect to all 2-subsets of vertices. A *subgraph* (*sub-digraph*) of a graph G (digraph $\mathcal{G}$) is a graph (digraph) with vertex and edge (arc) sets that are subsets of those of G. A subgraph *induced by a subset* $X \subset V$ in graph G (digraph $\mathcal{G}$) is a graph (digraph)

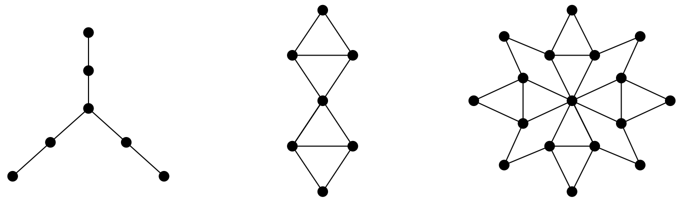


Figure 2.1: Pseudo regular graphs

with vertex set X, and edges (arcs) are those of G that have both endpoints in X. An induced subgraph isomorphic to a complete graph is called a *clique*. The complement of a clique is called *coclique*. A *supergraph* of a graph G is a graph that has G as a subgraph.

A *walk* in a graph G (digraph $\mathcal{G}$) is a sequence $v_0e_1v_1 \ldots v_{\ell-1}e_\ell v_\ell$, whose terms are alternately vertices and edges (arcs) of G ($\mathcal{G}$) which are not necessarily distinct, such that e_i is an edge (arc) starting at v_{i-1} and ending at v_i, $1 \leq i \leq \ell$. If $v_0 = v_\ell$ we call it a *closed walk*.

A *k-regular graph* is a graph where each of its vertices has the same number k of neighbors, i.e. each vertex is of degree k. A *k-regular digraph* is a digraph where each of its vertices has the same out-degree and in-degree equal to k. The adjacency matrix of a k-regular graph (digraph) has a constant row and column sum k. In general, we call matrices with constant row and column sum k, the *k-regular matrices*.

The 2-*degree* of a vertex v_i of a graph G, denoted by t_i, is the sum of the degrees of the vertices adjacent to v_i. The *average-degree* of v_i is t_i/d_i. The graph G is *k-pseudo regular* if each vertex v_i of G has average-degree

k ([26]). Any k-regular graph is k-pseudo regular, but the converse is not necessarily true. Figure 2.1 shows some examples of pseudo regular graphs.

A *path* in graph G (digraph $\mathcal{G}$) is a walk which contains no repeated vertices. A graph G (digraph $\mathcal{G}$) is *connected* (*weakly connected*) if from any vertex to any other vertex there is a path in G ($\mathcal{G}$). If G is not connected we call it a *disconnected* graph. The connected graph G is of *index* r if removal of $r+1$ edges results in a disconnected graph and r is the smallest number with this property. A digraph is *strongly connected* if for every pair u, v of vertices, there is a path from u to v and one from v to u. A *component* (*weak component*) of a graph (digraph) is a maximal connected subgraph (weakly connected sub-digraph). The *strong components* of a digraph are the maximal strongly connected sub-digraphs. Note that if $\mathcal{G}$ is a strongly connected digraph with n vertices and m arcs, then $n \leq m$.

2.2 Eigenvalues of a graph

The *characteristic polynomial* of a matrix A is the polynomial $\det(A - xI)$. The characteristic polynomial of the graph G is the characteristic polynomial of the adjacency matrix of the graph. We denote the characteristic polynomial of the graph G by $\Phi_G(x)$.

Theorem 1 [5] *If $G_1, G_2, \ldots, G_k$ are the components of the graph, we have*

$$\Phi_G(x) = \Phi_{G_1}(x)\Phi_{G_2}(x)\ldots\Phi_{G_k}(x)\ . \tag{2.1}$$

The formula (2.1) is also valid for the case of a digraph $\mathcal{G}$ and its strong components $\mathcal{G}_1, \mathcal{G}_2, \ldots, \mathcal{G}_k$.

The roots of the characteristic polynomial are the *eigenvalues* of A. A non-zero vector v is an *eigenvector* of A with eigenvalue λ if the equation $Av = \lambda v$ is satisfied. Note that an eigenvector cannot be the zero vector. Three useful properties of eigenvalues of a matrix are:

Theorem 2 [5] *Given a symmetric $n \times n$ matrix A with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$, we have the following*

1. (**Interlacing property**) [5] *If $B_{m\times m}$ is principal submatrix of A with eigenvalues $\mu_1 \geq \ldots \geq \mu_m$, we have $\lambda_k \geq \mu_k \geq \lambda_{n-m+k}$, for $k = 1, \ldots, m$;*

2. (**AM-QM Inequality**)[23] *Arithmetic mean is less than quadratic mean*

$$\frac{\lambda_1 + \lambda_2 + \ldots + \lambda_n}{n} \leq \sqrt{\frac{\lambda_1^2 + \lambda_2^2 + \ldots + \lambda_n^2}{n}}\ ; \tag{2.2}$$

3. (**Rayleigh's principle**) [1] *For a given vector $\mathbf{x}$, the Rayleigh quotient $R_A(\mathbf{x}) = \dfrac{\mathbf{x}A\mathbf{x}^t}{\mathbf{x}\mathbf{x}^t}$ satisfies*

$$\lambda_n \leq R_A(\mathbf{x}) \leq \lambda_1 \qquad (\text{for all nonzero } \mathbf{x} \in \mathbb{R}^n)\ . \tag{2.3}$$

If we choose an all-one vector $\mathbf{j} = [1\ 1 \cdots 1]$ and apply the Rayleigh's principle for matrix $A_{n\times n}$, then $\lambda_n \leq R_A(\mathbf{j}) = \dfrac{s}{n} \leq \lambda_1$, where s is the sum of all entries of A. The equality happens when A is regular with row sum $\dfrac{s}{n}$.

Theorem 3 [*11*] **(Schurs Unitary Triangularization Theorem)** *Given an $n \times n$ matrix A with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$, there is a unitary $n \times n$ matrix U such that $T = U^*AU$ is upper triangular and each diagonal element of T, t_{ii}, is equal to λ_i.*

A matrix is *normal* if it commutes with its conjugate transpose.

Theorem 4 [*11*] *Let A and B be normal matrices. If $AB = BA$ then there exists a unitary matrix U such that U^*AU and U^*BU are diagonal matrices.*

The *eigenvalue*(*s*) of a graph or digraph is (are) defined to be the eigenvalue(s) of its adjacency matrix. It is not hard to see that a graph G has only one eigenvalue if and only if G is an empty graph. The *spectral radius* of G is $r = \max\{|\lambda_i| : \lambda_i \text{ is an eigenvalue of } G\}$.
Note that since the adjacency matrix has zero on the diagonal, r is also an eigenvalue of G. The *spectrum* of a graph (digraph) is the multiset of eigenvalues of the graph. The spectra of some graphs are known. For example, for the complete graph K_n, the eigenvalues are $n-1$ (with multiplicity one) and -1 (with multiplicity $n-1$). For the star graph S_n, the eigenvalues are $\pm\sqrt{n-1}$ (each with multiplicity one) and 0 (with

multiplicity $n-2$). For the spectrum of the complete bipartite graph, we have the following useful lemma.

Lemma 2.2.1 [2] *The spectrum of the complete bipartite graph $K_{m,n}$ consists of $\pm\sqrt{mn}$ (each with multiplicity one) and 0 (with multiplicity $m+n-2$).*

PROOF. The adjacency matrix of $K_{m,n}$, A with order $(m+n)\times(m+n)$, is of the form

$$A = \begin{bmatrix} \mathbf{0}_{n\times n} & \mathbf{1}_{n\times m} \\ \mathbf{1}_{m\times n} & \mathbf{0}_{m\times m} \end{bmatrix}.$$

Define matrices $B_{2\times 2}$ and $S_{(m+n)\times 2}$ to be

$$B = \begin{bmatrix} 0 & m \\ n & 0 \end{bmatrix}, \quad S = \begin{bmatrix} \mathbf{1}_{n\times 1} & \mathbf{0}_{n\times 1} \\ \mathbf{0}_{m\times 1} & \mathbf{1}_{m\times 1} \end{bmatrix}.$$

It is straight forward that $AS = SB$. Now, if v is an eigenvector of matrix B for an eigenvalue λ, then Sv is an eigenvector of A for the same eigenvalue λ:

$$Bv = \lambda v \quad \Rightarrow \quad A(Sv) = ASv = SBv = S\lambda v = \lambda(Sv)$$

Now, B has eigenvalues $\pm\sqrt{mn}$, which are the nonzero eigenvalues of $K_{m,n}$. But the rank of A is 2 and so, the rest of the eigenvalues are 0. □

The method that we used in the above proof is called the *equitable partitions* ([2], page 28). Let A be a symmetric $n\times n$ matrix with rows and columns indexed by $I = \{1,\dots,n\}$. Suppose $\mathcal{I} = \{I_1,\dots,I_r\}$ is a partition of I, where $|I_j| = n_j$. Now, we partition A into blocks of size n_j according to $\mathcal{I}$:

$$A = \begin{bmatrix} A_{11} & \cdots & A_{1r} \\ \vdots & \ddots & \vdots \\ A_{r1} & \cdots & A_{rr} \end{bmatrix}.$$

If the row sum of each block A_{ij} is constant, the partition is called *equitable*. We define the *characteristic matrix* $S = [s_{ij}]$ to be the $n \times r$ matrix so that the rows are indexed by I and the columns are indexed by $\mathcal{I}$ and

$$s_{ij} = \begin{cases} 1, & i \in I_j \;; \\ 0, & \text{otherwise.} \end{cases}$$

Define the *quotient matrix* $B = [b_{ij}]$ to be the $r \times r$ matrix where b_{ij} is the average row sum of A_{ij}. In an equitable partition we have $A_{ij}\mathbf{1} = b_{ij}\mathbf{1}$ and therefore, $AS = SB$. $([2], \text{page } 28)$

Lemma 2.2.2 [2] *If the symmetric matrix A has an equitable partition $\mathcal{I}$, then the eigenvalues of the quotient matrix B are also the eigenvalues of A.*

PROOF. Suppose λ is an eigenvalue of B with the corresponding eigenvector v. Then $Bv = \lambda v$ implies

$$ASv = SBv = \lambda Sv$$

and therefore, Sv is an eigenvector of A with the eigenvalue λ. $\square$

There are also some more useful properties about the spectrum of a graph.

Proposition 2.2.1 [5] *Suppose G is a graph of order n with m edges and with eigenvalues $\lambda_1, \ldots, \lambda_n$. The following statements hold:*

1. *The numbers $\lambda_1, \ldots, \lambda_n$ are real and $\sum_{i=1}^{n} \lambda_i = 0$.*

2. *$\sum_{i=1}^{n} \lambda_i^2 = 2m$, $\sum_{i<j} \lambda_i \lambda_j = -m$, and so, if $m = 0$ we have $\lambda_1 = \ldots = \lambda_n = 0$.*

3. *If $m \geq 1$, and λ_1 is the greatest eigenvalue and λ_n is the smallest one, we have*

   (a) $1 \leq \lambda_1 \leq n-1$. *The upper bound holds if and only if G is a complete graph, and the lower bound is reached if and only if G is union of some K_2's and K_1's.*

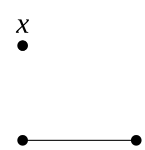
   (b) $-\lambda_1 \leq \lambda_n \leq -1$. *The upper bound is attained if and only if G is the union of complete graphs, and the lower bound holds if and only if a component of G having the greatest index is a bipartite graph.*

4. *G has two distinct eigenvalues if and only if G is the union of r_1 complete graphs of order $\lambda_1 + 1$, where r_1 is the multiplicity of λ_1. In this case, the other eigenvalue is -1 with multiplicity $r_1 \lambda_1$.*

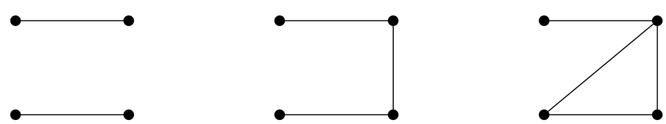
5. *Suppose $m \geq 1$. The spectrum of G, say S, is symmetric with respect to the zero point, i.e. for every $\lambda \in S$, $-\lambda$ is also in S with the same multiplicity, if and only if G is bipartite.*

Theorem 5 [5] *If the spectrum of graph G contains exactly one positive eigenvalue, then G is a complete multipartite graph plus some isolated vertices.*

PROOF. The isolated vertices would add some 0s to the spectrum of a graph. So, without loss of generality, we may ignore the isolated vertices. If G is not a complete multipartite graph, it has the subgraph below as an induced subgraph



But x is not an isolated vertex in G and so, G has at least one of the graphs H_1, H_2, or H_3 as an induced subgraph.



H_1 H_2 H_3

However, all these graphs have two positive eigenvalues, and therefore, by Theorem 2 (interlacing property), G has at least two positive eigenvalues. A contradiction. □

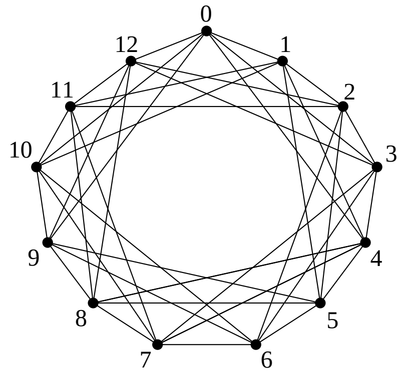


Figure 2.2: Paley graph of order 13

2.3 Strongly Regular Graphs

Definition 2.3.1 [7] A *strongly regular graph* (SRG) with parameters (n, k, λ, μ) is a k-regular graph of order n where every two adjacent vertices have the same number λ of neighbors in common, and every two non-adjacent vertices have the same number μ of neighbors in common.

The adjacency matrix A of an SRG with parameters (n, k, λ, μ) satisfies the equation

$$A^2 = kI_n + \lambda A + \mu(J_n - I_n - A), \tag{2.4}$$

where J_n is the $n \times n$ all-one matrix.

The *Paley graph* of order q, $q \equiv 1 (\mathrm{mod}\, 4)$ a prime power, is a graph P with q vertices such that two vertices are adjacent if their difference is a square in the finite field $\mathbb{F}_q$. Note that in order to have the adjacency matrix of a graph q must be 1 (mod 4). A Paley graph is, in fact, a strongly regular graph with parameters $(q, \frac{q-1}{2}, \frac{q-5}{4}, \frac{q-1}{4})$. The eigenvalues of a

Paley graph are $\frac{q-1}{2}, \frac{-1\pm\sqrt{q}}{2}$ with multiplicities $1, \frac{q-1}{2}, \frac{q-1}{2}$ respectively [18, 22]. Figure 2.2 shows the Paley graph of order 13 which is an SRG with parameters $(13,6,2,3)$.

The eigenvalues of a strongly regular graph with parameters (n,k,λ,μ) in general are known and consist of k (with multiplicity 1) and the two roots x_1, x_2 of the polynomial $x^2+(\mu-\lambda)x+(\mu-k)$ (with multiplicities r and s, calculated by solving the simultaneous equations $r+s=n-1$ and $k+rx_1+sx_2=0$).

We can extract SRGs from some types of matrices.

Definition 2.3.2 A *Hadamard matrix* is a square $(-1,1)$-matrix whose rows are mutually orthogonal, i.e. if H is a Hadamard matrix of order n, $HH^t=nI_n$, where I_n is the $n\times n$ identity matrix.

The order of a Hadamard matrix must be 1, 2, or a multiple of 4. A Hadamard matrix is called *graphical* if it is symmetric with constant diagonal 1. If H is a graphical Hadamard matrix of order n with 1 on the diagonal, $A_H=\dfrac{1}{2}(J_n-H)$ is the adjacency matrix of a graph.

One way to get new Hadamard matrices from old is to use the Kronecker product. The *Kronecker product* of matrices $A=[a_{ij}]_{m\times n}$ and B is a $p\times q$ matrix, denoted by $A\otimes B$, is the block matrix $C=[a_{ij}B]$. If H_1 is a Hadamard matrix of order n_1 and H_2 is a Hadamard matrix of order n_2, then $H_1\otimes H_2$ is a Hadamard matrix of order n_1n_2. The Kronecker product of two regular graphical Hadamard matrices gives another regular graphical Hadamard matrix.

If H is a k-regular (recall that matrices with constant row and column sum k are the k-regular matrices) and graphical Hadamard matrix with 1 on the diagonal, it is easy to see that A_H satisfies

$$A_H^2 = \frac{n-1k}{2} I_n + \frac{n-2k}{4}(J_n - I_n) \tag{2.5}$$

which shows that the associated graph G of A_H is a strongly regular graph with parameters $(n,(n-k)/2,(n-2k)/4,(n-2k)/4)$.

Definition 2.3.3 A *Bush-type* Hadamard matrix $H = (H_{ij})$ of order $n = 4k^2$, where H_{ij} is a $2k \times 2k$ block matrix, is a Hadamard matrix with the properties $H_{ii} = J_{2k}$, and $H_{ij}J_{2k} = J_{2k}H_{ij} = 0$, for $i \neq j$, $1 \leq i, j \leq 2k$.

Kharaghani [13] constructed a Bush-type Hadamard matrix of order n^2 from a Hadamard matrix of order n.

Theorem 6 [*13*] *If there exists a Hadamard matrix of order $n = 4k$, then there exists a Bush-type Hadamard matrix of order $n^2 = 16k^2$.*

PROOF. Suppose $H = [\mathbf{c}_1\ \mathbf{c}_2\ \ldots\ \mathbf{c}_n]$ is a Hadamard matrix of order n where $\mathbf{c}_i$s are columns of H so that the last column of H equals all-one matrix (this can be done by multiplying rows by -1). Define for $i = 1, \cdots, n$, $C_i = \mathbf{c}_i\mathbf{c}_i^t$. It is easy to see that the following are true:

1. For $i = 1, \cdots, n$, C_i is symmetric with diagonal 1.

2. For $i = 1, \cdots, n-1$, C_i has row and column sums equal to 0.

3. $C_iC_j = 0$ if $i \neq j$, $1 \leq i, j \leq n$.

4. $C_1^2 + C_2^2 + \ldots + C_n^2 = nHH^t = n^2 I_n$.

Now, consider a Latin square $A = [a_{ij}]$ such that for $1 \leq i, j \leq n$, $a_{ij} = j + n - i \pmod{n}$. We obtain a Bush-type Hadamard matrix of order n^2 by replacing each entry i of A by matrix C_i. $\square$

Chapter 3

Energy of Graphs

In this section we outline a few results on the energy of graphs. One of the long known results is the Coulson Integral formula for the graph energy.

Theorem 7 [8] *Let G be a graph with n vertices and $\Phi_G(x)$ be the characteristic polynomial of G. Then*

$$\mathcal{E}(G) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\left(n - \frac{ix\Phi'_G(ix)}{\Phi_G(ix)}\right)dx\ ,$$

where $\Phi'_G(x) = \frac{d}{dx}\Phi_G(x)$ and $i = \sqrt{-1}$.

PROOF. Let $\lambda_1 \geq \ldots \geq \lambda_n$ be all the eigenvalues of the graph G and let z be a complex variable. $\Phi_G(z) = \prod_{i=1}^{\ell}(z-\nu_i)^{n_i}$, where $\sum_{i=1}^{\ell} n_i = n$ and ν_i's are distinct eigenvalues of G. Now, we have

$$\frac{\Phi'_G(z)}{\Phi_G(z)} = \frac{\sum_{i=1}^{\ell}\left(n_i(z-\nu_i)^{n_i-1}\prod_{j\neq i}(z-\nu_j)^{n_j}\right)}{\prod_{i=1}^{\ell}(z-\nu_i)^{n_i}} = \sum_{i=1}^{\ell}\frac{n_i}{z-\nu_i}\ .$$

Therefore, $\Phi'_G(x)/\Phi_G(x)$ is an analytic function with only ℓ simple poles, $\nu_1,\cdots,\nu_\ell$. Choose $r \geq \lambda_1$. Let Γ (Figure 3.1) be the contour that goes along the y-axis from the point $(0,r)$ to point $(0,-r)$ and returns to $(0,r)$ through a semicircle with radius r. Note that only positive ν_i's are interior

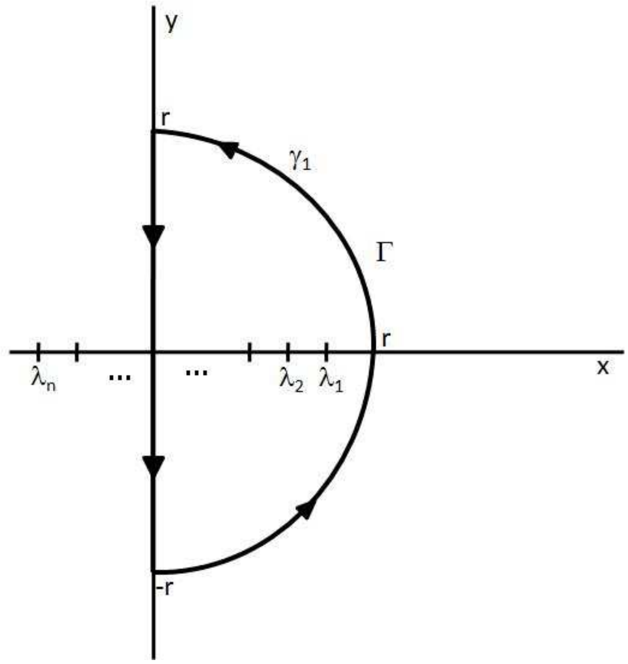


Figure 3.1: Contour Γ

to the contour Γ. Now, define the function

$$f(z) := z\frac{\Phi'_G(z)}{\Phi_G(z)} = \sum_{i=1}^{\ell} \frac{n_i z}{z-\nu_i}$$

and apply the Cauchy integral formula to it. We get

$$\frac{1}{2\pi i}\oint_\Gamma f(z)dz = \frac{1}{2\pi i}\oint_\Gamma \sum_{i=1}^{\ell} \frac{n_i z}{z-\nu_i}dz = \frac{1}{2\pi i}\sum_{i=1}^{\ell}\oint_\Gamma \frac{n_i z}{z-\nu_i}dz$$

$$= \sum_{+} n_i \nu_i = \sum_{+} \lambda_i = \frac{1}{2}\mathcal{E}(\mathcal{G}) \tag{3.1}$$

where $\sum_+$ is taken over the positive eigenvalues. The last equality in (3.1) comes from the fact that $\sum_{i=1}^{n} \lambda_i = 0$.

Since n is constant,

$$\frac{1}{2\pi i}\oint_\Gamma f(z)dz = \frac{1}{2\pi i}\oint_\Gamma [f(z)-n]dz$$

Let γ_1 be the semicircle in the contour Γ. We have

$$\int_{\gamma_1}[f(z)-n]dz = \int_{\gamma_1}\sum_{j=1}^{\ell}[\frac{n_j z}{z-\nu_j}-n_j]dz = \int_{\gamma_1}\sum_{j=1}^{\ell}\frac{n_j\nu_j}{z-\nu_j}dz \quad (\text{since } \sum_{j=1}^{\ell} n_j = n)$$

$$= \sum_{j=1}^{\ell} n_j\nu_j \int_{\gamma_1}\frac{1}{z-\nu_j}dz = \sum_{j=1}^{\ell} n_j\nu_j \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{ire^{it}}{re^{it}-\nu_j}dt$$

and

$$\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{ire^{it}}{re^{it}-\nu_j}dt = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} idt + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{i\nu_j}{re^{it}-\nu_j}dt = \pi i + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{i\nu_j}{re^{it}-\nu_j}dt\ .$$

If $r \to +\infty$, we have $\int_{\gamma_1}\frac{1}{x-\nu_j}dx = \pi i$ and therefore

$$\int_{\gamma_1}\sum_{j=1}^{\ell}\frac{n_j\nu_j}{x-\nu_j}dx = \pi i \sum_{j=1}^{\ell} n_j\nu_j = 0.$$

Thus,

$$\frac{1}{2}\mathcal{E}(\mathcal{G}) = \frac{1}{2\pi i}\oint_\Gamma [f(z)-n]dz = \frac{1}{2\pi}\int_{+\infty}^{-\infty}[f(iy)-n]dy = \frac{1}{2\pi}\int_{-\infty}^{+\infty}[n-f(iy)]dy$$

and the result follows. $\square$

The Coulson formula states that the energy of a graph depends on its characteristic polynomial. In chemistry, this formula shows that the energy of a molecule solely depends on its structure.

Coulson formula is perhaps the only theorem which gives an exact formula for finding the energy of a graph and yet the formula is fairly complicated. There are some lower and upper bounds for the energy of graphs which only depend on the number of vertices and edges. One of the well-known bounds is the McClelland bound.

Theorem 8 [*8*] (**McClelland, 1971**) *Consider a graph G of order n with m edges. Let A be its adjacency matrix. We have*

$$\sqrt{2m+n(n-1)|det(A)|^{\frac{2}{n}}} \leq \mathcal{E}(G) \leq \sqrt{2mn}. \tag{3.2}$$

PROOF. Let $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$ be the eigenvalues of G. Let μ be the arithmetic mean of the $\dfrac{n(n-1)}{2}$ distinct terms $|\lambda_i||\lambda_j|$ $(i<j)$, i.e.

$$\mu = \frac{2\sum_{i<j}|\lambda_i||\lambda_j|}{n(n-1)} ,$$

and η is the geometric mean of the terms $|\lambda_i||\lambda_j|$ $(i<j)$, i.e.

$$\eta = \left(\prod_{i<j}|\lambda_i||\lambda_j|\right)^{\frac{2}{n(n-1)}}$$

$$= \left(\prod_{i=1}^{n}|\lambda_i|^{n-1}\right)^{\frac{2}{n(n-1)}} = \left(\prod_{i=1}^{n}|\lambda_i|\right)^{\frac{2}{n}} = |\det A|^{\frac{2}{n}} .$$

Now, by Proposition 2.2.1

$$\mathcal{E}^2(G) = \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 = \sum_{i=1}^{n} |\lambda_i|^2 + 2\sum_{i<j} |\lambda_i||\lambda_j| = 2m + n(n-1)\mu\ .$$

Using the fact that the arithmetic mean of non-negative numbers is always greater than their geometric mean, we get the lower bound in (3.2). For the upper bound in (3.2), note that on one hand $\sum_{i=1}^{n}\sum_{j=1}^{n}(|\lambda_i| - |\lambda_j|)^2$ is always a non-negative quantity; on the other hand

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(|\lambda_i| - |\lambda_j|)^2 = \sum_{j=1}^{n}\sum_{i=1}^{n}|\lambda_i|^2 + \sum_{i=1}^{n}\sum_{j=1}^{n}|\lambda_j|^2 - 2(\sum_{i=1}^{n}|\lambda_i|)(\sum_{j=1}^{n}|\lambda_j|)$$

$$= 2mn + 2mn - 2\mathcal{E}^2(G)$$

Therefore, $4mn - 2\mathcal{E}^2(G) \geq 0$ and the result follows. $\square$

3.1 Minimal energy graphs

Many results on the minimal energy have been obtained for various classes of graphs. One of the very well-known results is the following theorem.

Theorem 9 [8] *Let G be a graph with m edges, then*

$$\mathcal{E}(G) \geq 2\sqrt{m}$$

with the equality attained if and only if G is a complete bipartite graph plus some isolated vertices.

PROOF.

$$\mathcal{E}^2(G) = \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 = \sum_{i=1}^{n} |\lambda_i|^2 + 2\sum_{i<j} |\lambda_i||\lambda_j|$$

$$\geq 2m + 2\left|\sum_{i<j} \lambda_i\lambda_j\right| \quad \text{(Triangle inequality)}$$

$$= 2m + 2m = 4m \quad \text{(Proposition 2.2.1)}$$

The equality happens if and only if the graph has exactly one positive and exactly one negative eigenvalue. This happens if and only if G is a complete bipartite graph plus some isolated vertices (by using Theorem 5). □

Now, if we want to find a bound which depends only on the number of vertices, we may restrict ourselves to graphs without isolated vertices.

Theorem 10 [8] *Let G be a graph of order n with no isolated vertices. We have*

$$\mathcal{E}(G) \geq 2\sqrt{n-1}.$$

The equality holds if and only if G is the star graph S_n.

PROOF. If G is connected, then it has at least $n-1$ edges and the theorem is a result of Theorem 9. Let G be disconnected with ℓ components, $G_1, \cdots, G_\ell$ with $n_1, \cdots, n_\ell$ vertices, respectively. We can apply the theorem for each connected component:

$$\mathcal{E}(G_i) \geq 2\sqrt{n_i - 1} \quad (\text{for } i = 1, \cdots, \ell)$$

Thus,

$$\mathcal{E}(G) = \sum_{i=1}^{\ell} \mathcal{E}(G_i) \geq 2\sum_{i=1}^{\ell} \sqrt{n_i - 1} = 2\sqrt{\left(\sum_{i=1}^{\ell} \sqrt{n_i - 1}\right)^2}$$

$$= 2\sqrt{\sum_{i=1}^{\ell}(n_i - 1) + 2\sum_{i<k} \sqrt{n_i - 1}\sqrt{n_k - 1}}$$

$$\geq 2\sqrt{n - \ell + \ell(\ell - 1)} \qquad\qquad (\text{since } n_i \geq 2)$$

$$= 2\sqrt{n - 1 + (\ell - 1)^2} \geq 2\sqrt{n - 1}$$

Note that there are $\ell(\ell-1)/2$ summands of the form $\sqrt{n_i - 1}\sqrt{n_k - 1}$.

$\square$

Therefore, among graphs of order n, the star graph S_n has the minimal energy. In [4], Caporossi et al by doing series of experiments and computations made a conjecture for the minimum energy graphs.

Conjecture 3.1.1 [4] *Connected graphs with minimum energy and $n \geq 6$ vertices and $n - 1 \leq m \leq 2(n-2)$ edges are stars with $m - n + 1$ additional edges for $m \leq n + (n-7)/2$* [*these additional edges are all connected to the same vertex*], *and bipartite graphs with two vertices on one side, one of which is connected to all vertices on the other side for $m > n + (n-7)/2$.*

The conjecture is proved to be true for $m = n-1, 2(n-2)$ in the same paper [4]. In [12] the conjecture is proved for $m = n$, and in [16] the second part of the conjecture on bipartite graphs is proved completely. Yet the conjecture is still open in the general case.

3.2 Maximal Energy Graphs

Since the energy of a graph can be used to approximate the total π-electron energy of the molecule, it has been intensively studied by many scholars. One of the most significant result is the upper bound obtained by Koolen and Moulton in [14]. In fact, they found the upper bound $\frac{n(1+\sqrt{n})}{2}$ for the energy of a graph of order n and characterized the maximal energy graph attaining this bound. Here, we review some of their results.

Theorem 11 *[14] Let G be a graph of order n with m edges. If $2m \geq n$, then*

$$\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}\,, \tag{3.3}$$

and equality is attained if and only if G is K_n, $\frac{n}{2}K_2$, or a strongly regular graph with two eigenvalues which both have the absolute value $\sqrt{\frac{2m-(2m/n)^2}{n-1}}$.

PROOF. Let $\lambda_1 \geq \ldots \geq \lambda_n$ be the eigenvalues of G. Theorem 2(2) shows that $\lambda_1 \geq \frac{2m}{n}$ and from Proposition 2.2.1(2) we have $\sum_{i=1}^{n} \lambda_i^2 = 2m$. Therefore,

$$\sum_{i=2}^{n} \lambda_i^2 = 2m - \lambda_1^2, \quad \lambda_1^2 \leq 2m.$$

Applying Cauchy-Schwartz inequality to the vectors $(|\lambda_2|,\ldots,|\lambda_n|)$ and $(1,1,\ldots,1)$ with $n-1$ entries, we get

$$\sum_{i=2}^{n}|\lambda_i| \le \sqrt{(n-1)(\sum_{i=2}^{n}|\lambda_i|^2)} = \sqrt{(n-1)(2m-\lambda_1^2)}. \tag{3.4}$$

Since $\lambda_1 \ge 0$, $\mathcal{E}(G) \le \lambda_1 + \sqrt{(n-1)(2m-\lambda_1^2)}$. Now, using the fact that the function $F(x) := x + \sqrt{(n-1)(2m-x^2)}$ is decreasing on the interval $\sqrt{2m/n} < x \le \sqrt{2m}$ and that $\sqrt{2m/n} \le 2m/n \le \lambda_1$ (since $2m \ge n$), we have $F(\lambda_1) \le F(2m/n)$ and so, inequality (3.3) holds.

Since $\mathcal{E}(\frac{n}{2}K_2) = n$ and $\mathcal{E}(K_n) = 2n-2$, if graph G is either $\frac{n}{2}K_2$ or K_n the equality hold in (3.3).

If equality holds in (3.3), then λ_1 must be $2m/n$. Therefore G should be regular of degree $2m/n$. Also, the equality must hold in (3.4), and we have $|\lambda_i| = \sqrt{\frac{(2m-(2m/n)^2)}{n-1}}$ for $2 \le i \le n$. So, we have three possibilities:

1. G is $\frac{n}{2}K_2$. Its eigenvalues are ± 1 (both with multiplicity $\frac{n}{2}$);
2. G is K_n. Its eigenvalues are $n-1$ (with multiplicity 1) and -1 (with multiplicity $n-1$);
3. G is a non-complete connected strongly regular graph with three eigenvalues having distinct absolute values equal to $2m/n$ or $\sqrt{(2m-(2m/n)^2)/(n-1)}$.

This completes the proof. $\square$

Note that Theorem 11 is an improvement on the McCelland bound. In fact, for the function $F(x)$ in the proof we have $F(\sqrt{2m/n}) = \sqrt{2mn}$.

Since F decreases on the interval $\sqrt{2m/n} < x \leq \sqrt{2m}$, we have

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

and the equality holds if and only if $2m = n$ and $G = (n/2)K_2$.

Theorem 12 [14] *Let G be a graph with n vertices. Then*

$$\mathcal{E}(G) \leq \frac{n(1+\sqrt{n})}{2} \tag{3.5}$$

and equality holds if and only if G is a strongly regular graph with parameters

$$(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+2\sqrt{n})/4). \tag{3.6}$$

PROOF. Suppose G has m edges and $2m \geq n$. In Theorem 11, consider the left hand side of the inequality (3.3) as a function of m. It is maximized when $m = \frac{n^2+n\sqrt{n}}{4}$. Then on replacing m in inequality (3.3) by $\frac{n^2+n\sqrt{n}}{4}$, we obtain the inequality (3.5). By Theorem 11, the equality holds if and only if G is a strongly regular graph with parameters $(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+2\sqrt{n})/4)$.

If $2m < n$ then G has at least $n-2m$ isolated vertices. Let $\tilde{G}$ be a graph obtained from G by deleting the $n-2m$ isolated vertices. Therefore, $\tilde{G}$ is a graph with $2m$ vertices and m edges. By Theorem 11, $\mathcal{E}(\tilde{G}) \leq 2m \leq n \leq \dfrac{n}{2}(1+\sqrt{n})$. Since $\mathcal{E}(G) = \mathcal{E}(\tilde{G})$, the proof is complete. $\square$

In fact, as Nikiforov later proved in [18], for a given $\varepsilon > 0$ there exists a graph G of order n such that for sufficiently large $n \geq 1$, $\mathcal{E}(G) \geq (1-\varepsilon)\frac{n}{2}(\sqrt{n}+1)$.

Theorem 13 [*18*] *For all sufficiently large n, there exists a graph G of order n such that* $\mathcal{E}(G) \geq \frac{n}{2}(\sqrt{n} - n^{1/10})$.

PROOF. Let m be the number of edges in G and let $|\lambda_1| \geq |\lambda_2| \geq ... \geq |\lambda_n|$ be the eigenvalues of G. By using property 2 of Proposition 2.2.1 we have

$$2m - |\lambda_1|^2 = |\lambda_2|^2 + \ldots + |\lambda_n|^2 \leq |\lambda_2|^2 + |\lambda_2||\lambda_3| + \ldots + |\lambda_2||\lambda_n|$$

$$\leq |\lambda_2|(\mathcal{E}(G) - |\lambda_1|).$$

Therefore, if $m > 0$ we have

$$\mathcal{E}(G) \geq |\lambda_1| + \frac{2m - |\lambda_1|^2}{|\lambda_2|} . \tag{3.7}$$

First, we prove the theorem for a prime $p > 11$ so that $p \equiv 1 \pmod 4$. Consider $P(p)$, the Paley graph of order p. Recall from page 19 that the Paley graph is in fact strongly regular with parameters $(p, (p-1)/2, (p-5)/4, (p-1)/4)$, the number of edges $\frac{p(p-1)}{4}$, the largest eigenvalue $\lambda_1 = \frac{p-1}{2}$, and the second largest eigenvalue $|\lambda_2| = |\frac{-1-p^{\frac{1}{2}}}{2}| = \frac{1+p^{\frac{1}{2}}}{2}$. Therefore, by (3.7) we have

$$\mathcal{E}(P(p)) \geq \frac{p-1}{2} + \frac{2p(p-1)/4 - (p-1)^2/4}{(1+p^{\frac{1}{2}})/2}$$

$$\geq \frac{p-1}{2}\left(1+\frac{p+1}{1+p^{\frac{1}{2}}}\right)=\frac{p^{\frac{3}{2}}+p^{\frac{1}{2}}-2}{2}>\frac{p^{\frac{3}{2}}}{2}\ .$$

Consequently, the theorem is true for a prime $p \equiv 1\,(\mathrm{mod}\,4)$.

In the general case, for a sufficiently large n, there exists a prime $p \equiv 1\,(\mathrm{mod}\,4)$ such that $n \leq p \leq n+n^{\frac{11}{20}+\varepsilon}$. For a large n, fix a prime p such that $p \leq n+n^{\frac{3}{5}}/2$ and consider the Paley graph, $P(p)$, of order p with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_p$. Let K be a set of n vertices in $P(p)$ and consider the subgraph $P_K(n)$ of $P(p)$ induced by K. The average number of edges, m_K, in $P_K(n)$ is obtained as follows

$$\frac{m_K}{m}=\frac{n(n-1)/2}{p(p-1)/2}\ \Rightarrow\ m_K=\frac{n(n-1)}{p(p-1)}m=\frac{n(n-1)}{4}\ .$$

Therefore, we may pick the vertices K such that the number of edges of $P_K(n)$ is greater than or equal to $n(n-1)/4$. Let $\mu_1 \geq \ldots \geq \mu_n$ be the eigenvalues of $P_K(n)$. By the interlacing property (page 12), we know that $\mu_1 \leq \lambda_1$ and $\mu_2 \leq \lambda_2$. Therefore,

$$\mathcal{E}\left(P_K(n)\right) \geq |\mu_1|+\frac{2m-|\mu_1|^2}{|\mu_2|} \geq \frac{n-1}{2}+\frac{n(n-1)/2-|\lambda_1|^2}{|\lambda_2|}$$

$$\geq \frac{n-1}{2}+\frac{n(n-1)/2-(n+n^{\frac{3}{5}}/2-1)^2/4}{((n+n^{\frac{3}{5}}/2)^{\frac{1}{2}}+1)/2}$$

$$> \frac{n-1}{2}+\frac{n(n-1)/2-(n+n^{\frac{3}{5}}/2)^2/4}{((n+n^{\frac{3}{5}}/2)^{\frac{1}{2}}+1)/2} > \frac{n^{\frac{3}{2}}}{2}-n^{\frac{11}{10}}\ .$$

□

An SRG with parameters (3.6) is called a *max energy graph* of order n. In [9] and [10], a max energy graph of order $4m^4$ for any positive integer m has been found. In fact, as we will see below, the regular graphical Hadamard matrices lead us to the max energy graphs.

Recall that a Hadamard matrix H is k-regular if all its row and column sums are constant k, and it is graphical if it is symmetric with constant diagonal δ. Following [9] we call H of *type* $+1$ if $\delta k > 0$ and of *type* -1 if $\delta k < 0$.

Recall that we can associate a graph G to the graphical Hadamard matrix H so that $A_H = \frac{1}{2}(J_n - \delta H)$ is its adjacency matrix. Let ρ be the type of the regular graphical Hadamard matrix H of order n. Then $\delta k = \rho\sqrt{n}$ and the associated graph G is regular of degree $(n-\delta k)/2 = (n-\rho\sqrt{n})/2$. Since H is graphical and therefore symmetric, we have $HH^t = H^2 = nI_n$ and $J_nH = HJ_n$. Also, since H is regular, $J_nH = HJ_n = kJ_n$. Now, we have

$$A_H^2 = \left[\frac{1}{2}(J_n - \delta H)\right]\left[\frac{1}{2}(J_n - \delta H)\right] = \frac{1}{4}\left[J_n^2 - \delta J_n H - \delta H J_n + \delta^2 H^2\right]$$

$$= \frac{1}{4}\left[nJ_n - 2\delta k J_n + \delta^2 n I_n\right] = \frac{n-\delta k}{2} I_n + \frac{n-2\delta k}{4}(J_n - I_n).$$

Therefore, by formula (2.4), G is a strongly regular graph with parameter set

$$\left(n, \frac{n-\rho\sqrt{n}}{2}, \frac{n-2\rho\sqrt{n}}{4}, \frac{n-2\rho\sqrt{n}}{4}\right).$$

As we see the regular graphical Hadamard matrices of type -1 give max energy graphs.

Consider the following matrix:

$$H_+ = \begin{bmatrix} 1 & 1 & 1 & - \\ 1 & 1 & - & 1 \\ 1 & - & 1 & 1 \\ - & 1 & 1 & 1 \end{bmatrix}$$

The Kronecker product of H_+ with any regular graphical Hadamard matrix of order n of type -1 gives a regular graphical Hadamard matrix of type -1 of order $4n$. Haemers in [9], by making a slight change in the construction of Theorem 6, found a regular graphical Hadamard matrix of type -1:

Theorem 14 ([9], [13]) *If n is the order of a Hadamard matrix, then there exist regular graphical Hadamard matrices of order n^2 of type -1, and therefore max energy graphs of order n^2.*

PROOF. Let $H = [\mathbf{c}_1\ \mathbf{c}_2\ \dots\ \mathbf{c}_n]$ be a Hadamard matrix of order n where $\mathbf{c}_i$s are columns of H so that the last column of H equals all-one. Define for $i = 1, \dots, n-1$, $C_i = \mathbf{c}_i\mathbf{c}_i^t$. So, C_i ($i = 1, \dots, n-1$) is symmetric with diagonal 1 and with row and column sums equal to 0. Let $C_n = -J_n$. It is easy to see that the following are satisfied:

1. $C_iC_j = 0$ if $i \neq j$, $1 \leq i, j \leq n$

2. $C_1^2 + C_2^2 + \ldots + C_n^2 = nHH^t = n^2 I_n$

Now, consider the matrix $A = [a_{ij}]$, a symmetric Latin square with entries $1, \ldots, n$ with constant diagonal 1. Let H' be the Hadamard matrix of order n^2 which is obtained by replacing each entry i of A with matrix C_i. H' is symmetric and has constant diagonal 1. It is also a -4-regular Hadamard matrix. Therefore, H' is the regular graphical Hadamard matrix of order n^2 of type -1. $\square$

Yu et al. found a better upper bound for the graph energy in [26]. Recall that the sum of the degrees of the vertices adjacent to the vertex v_i is its 2-degree, denoted by t_i, and t_i/d_i is its average-degree. If all vertices of the graph G have average-degree k, G is k-pseudo regular.

Theorem 15 [26] *For the graph G of order n, with m edges, if we have the degree sequence $d_1, d_2, \cdots, d_n$ and 2-degree sequence $t_1, t_2, \cdots, t_n$, then*

$$\mathcal{E}(G) \leq \sqrt{\left(\sum_{i=1}^{n} t_i^2\right) / \left(\sum_{i=1}^{n} d_i^2\right)} + \sqrt{(n-1)\left(2m - \left(\sum_{i=1}^{n} t_i^2\right) / \left(\sum_{i=1}^{n} d_i^2\right)\right)}.$$

The equality is attained if and only if G is K_n, $\frac{n}{2}K_2$, or a non-bipartite connected k-pseudo regular graph ($k > \sqrt{2m/n}$) with three distinct eigenvalues k, $-\sqrt{(2m-k^2)/(n-1)}$, and $\sqrt{(2m-k^2)/(n-1)}$.

The argument made in [26] for the proof of Theorem 15 is similar to the proof of Theorem 11 except for the bound for λ_1 they used

$\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^{n} t_i^2}{\sum_{i=1}^{n} d_i^2}}$ (found in [25]) where the equality happens if and only if the graph is a non-bipartite pseudo regular graph. Although the bound attained in Theorem 15 is better than Koolen and Moulton bound, there are not known examples different from those of Koolen and Moulton's which attain this newer bound and do not satisfy the conditions of Theorem 12.

3.3 Hyper-energetic Graphs

In summer 2008, I had a chance to work with Lily Liu, who was one of my supervisor's summer students. Part of the work in this section resulted from the discussion we had with our supervisor.

In searching for maximum energy graphs we see that by using the interlacing property (Theorem 2), the energy of an induced subgraph of a graph G is less than the energy of G. This is not true for an arbitrary subgraph of a graph G unless it is induced. For example, the energy of C_4 is less than the energy of $C_4 - \{e\} = P_4$. In fact, $\mathcal{E}(C_4) = 4 < 2\sqrt{5} = \mathcal{E}(P_4)$ ([6]). Based on this property, Gutman in 1978 made a conjecture that among graphs of order n, the complete graph K_n has the maximum energy. The conjecture was soon rejected and it was shown that, in fact, there exist subgraphs of K_n with energy greater than that of K_n. These graphs are called *hyper-energetic* graphs.

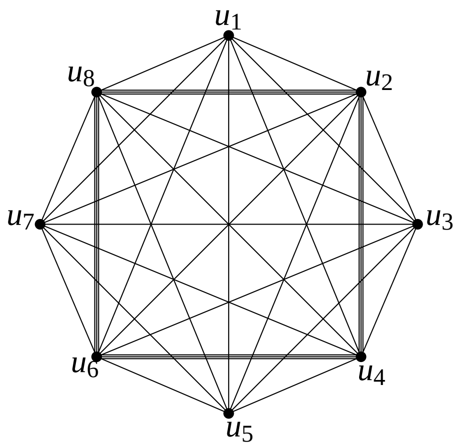


Figure 3.2: A hyper-energetic graph on 8 vertices

Definition 3.3.1 A graph G with n vertices is said to be *hyper-energetic* if its energy $\mathcal{E}(G)$ satisfies the inequality $\mathcal{E}(G) > 2n-2$.

Here is an example of a hyper-energetic graph:

EXAMPLE. Consider K_8; we know that $\mathcal{E}(K_8) = 14$. Now delete the edges of a quadrangle of K_8, say u_2u_4, u_4u_6, u_6u_8, and u_8u_2 (see Figure 3.2). The incidence matrix of such a graph is

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

The characteristic polynomial of this graph is

$$\phi(\lambda) = (\lambda^2 - 4\lambda - 13)(\lambda+1)^5(\lambda-1)$$

and the eigenvalues are $2+\sqrt{17},\ 2-\sqrt{17},\ -1,\ -1,\ -1,\ -1,\ -1,\ 1.$ Therefore,

$$\mathcal{E}\left(K_8-u_2u_4-u_4u_6-u_6u_8-u_8u_2\right)=2\sqrt{17}+5+1>14=\mathcal{E}\left(K_8\right).$$

As it is mentioned in the Theorem 12, only those strongly regular graphs with parameters (3.6) give the maximal energy.

Here we consider another class of strongly regular graphs with parameters $(n,(n-1)/2,(n-5)/4,(n-1)/4)$ which are called *conference graphs*. In [15], it is shown that these graphs are in fact hyper-energetic graphs.

Definition 3.3.2 A *conference matrix* C is an $n\times n$ $(0,\pm 1)$-matrix with zero diagonal satisfying $CC^t=(n-1)I_n$.

It can be shown that a necessary condition for existence of a symmetric conference matrix of order n is $n\equiv 2 \pmod 4$ ([24]). Let $q\equiv 1 \pmod 4$ be a prime power and consider the index set $I=\mathbb{F}_q\cup\{\infty\}$. Define the matrix $C=[c_{ij}]$ so that the rows and columns are indexed by I and

$$c_{ij}=\begin{cases} 1, & \text{if } i,j\in\mathbb{F}_q,\ i-j\in S_q\\ -1, & \text{if } i,j\in\mathbb{F}_q,\ i-j\in N_q\\ 1, & \text{if } i=\infty \text{ or } j=\infty \text{ but not both}\\ 0, & \text{if } i=j \end{cases}$$

where S_q is the set of squares and N_q is the set of non-squares of $\mathbb{F}_q$.

It is proved in [24] that C with the construction above is a symmetric Conference matrix of order $q+1$.

EXAMPLE. The following matrix is a conference matrix of order 14.

$\mathbb{F}_{13} = \mathbb{Z}_{13}$, $S_{13} = \{1,3,4,9,10,12\}$, and $N_{13} = \{2,5,6,7,8,11\}$.

$$C = \begin{bmatrix}
0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & 1 & - & 1 & 1 & - & - & - & - & 1 & 1 & - & 1 \\
1 & 1 & 0 & 1 & - & 1 & 1 & - & - & - & - & 1 & 1 & - \\
1 & - & 1 & 0 & 1 & - & 1 & 1 & - & - & - & - & 1 & 1 \\
1 & 1 & - & 1 & 0 & 1 & - & 1 & 1 & - & - & - & - & 1 \\
1 & 1 & 1 & - & 1 & 0 & 1 & - & 1 & 1 & - & - & - & - \\
1 & - & 1 & 1 & - & 1 & 0 & 1 & - & 1 & 1 & - & - & - \\
1 & - & - & 1 & 1 & - & 1 & 0 & 1 & - & 1 & 1 & - & - \\
1 & - & - & - & 1 & 1 & - & 1 & 0 & 1 & - & 1 & 1 & - \\
1 & - & - & - & - & 1 & 1 & - & 1 & 0 & 1 & - & 1 & 1 \\
1 & 1 & - & - & - & - & 1 & 1 & - & 1 & 0 & 1 & - & 1 \\
1 & 1 & 1 & - & - & - & - & 1 & 1 & - & 1 & 0 & 1 & - \\
1 & - & 1 & 1 & - & - & - & - & 1 & 1 & - & 1 & 0 & 1 \\
1 & 1 & - & 1 & 1 & - & - & - & - & 1 & 1 & - & 1 & 0
\end{bmatrix}$$

This conference matrix is a *normalized* Conference matrix since all entries in its first row and first column are 1 (except the $(1,1)$ entry which is 0). If we remove the first row and first column and change the "-" to "0", we get the adjacency matrix for the Conference graph of order 13. This Conference graph is in fact the Paley graph in Figure 2.2.

By constructing the Conference graphs from Conference matrices, we realize that these graphs are strongly regular graphs with parameters

$(4t+1, 2t, t-1, t)$, for every prime power t.

Let G_C be a conference graph of order $n = 4t+1$ with parameters $(4t+1, 2t, t-1, t)$. Using the argument made on page 18, we find the eigenvalues of G_C as follows:

$$\lambda_1 = 2t \qquad \text{(with multiplicity 1)}$$

$$\lambda_2 = \frac{-1+\sqrt{4t+1}}{2} \qquad \text{(with multiplicity 2t)}$$

$$\lambda_3 = \frac{-1-\sqrt{4t+1}}{2} \qquad \text{(with multiplicity 2t)}$$

Therefore the energy of G_C is:

$$\mathcal{E}(G_C) = 2t(1+\sqrt{4t+1}) = \frac{1}{2}(n-1)(1+\sqrt{n})$$

Since $n \geq 5$, it shows that $\mathcal{E}(G_C) \geq 2(n-1)$ and, therefore, we have the following.

Theorem 16 [*15*] *Conference graphs are hyper-energetic.*

We do not restrict ourselves to the strongly regular graphs, instead we may think of graphs which have the property for some of their vertices. Here we consider $\mu = \lambda$.

Definition 3.3.3 A graph G of order n is *locally strongly regular* (LSR) with parameters (n, k, λ) if it is regular of degree k and there exists at least one vertex such that it has λ common neighbors with every other vertices of G.

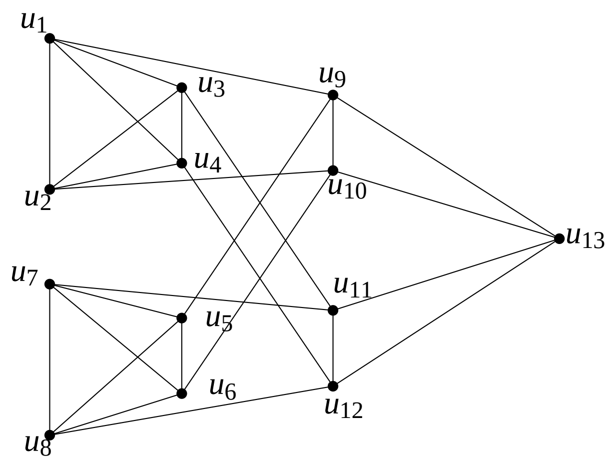


Figure 3.3: G_2

EXAMPLE. G_2 is an example of a locally strongly regular graph with parameters $(13, 4, 1)$ (Figure 3.3). It is a 4-regular graph with 13 vertices and u_{13} has the LSR property. With the labeling shown in Figure 3.3, the adjacency matrix of G_2 is

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

$$= \begin{bmatrix} J_4 - I_4 & \mathbf{0}_{4\times 4} & I_4 & \mathbf{0}_{4\times 1} \\ \mathbf{0}_{4\times 4} & J_4 - I_4 & I_4 & \mathbf{0}_{4\times 1} \\ I_4 & I_4 & \bigoplus_2 J_2 - I_2 & \mathbf{1}_{4\times 1} \\ \mathbf{0}_{1\times 4} & \mathbf{0}_{1\times 4} & \mathbf{1}_{1\times 4} & 0 \end{bmatrix}$$

In order to find the characteristic polynomial of the above matrix we have to find the determinant (3.8). The following transformations leave the value of (3.8) unchanged.

$$\begin{vmatrix} -x & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & -x & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & -x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & -x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -x & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -x & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & -x & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & -x & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -x & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -x & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -x & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -x & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & -x \end{vmatrix} \tag{3.8}$$

Add the first 12 rows to the last row and extract the factor $(-x+4)$ from the determinant to get (3.9).

$$= (-x+4)\begin{vmatrix} -x & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & -x & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & -x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & -x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -x & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -x & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & -x & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & -x & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -x & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -x & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -x & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -x & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{vmatrix} \tag{3.9}$$

Now, let $z = -x-1$. Subtract the last column from all the other columns;

then subtract the last row from from rows $9,10,11,12$ to get

$$(-x+4)\begin{vmatrix} -x & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & -x & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & -x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & -x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -x & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -x & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & -x & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & -x & 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & -1 & -1 & 0 & -1 & -1 & -1 & z & 0 & -1 & -1 & 0 \\ -1 & 0 & -1 & -1 & -1 & 0 & -1 & -1 & 0 & z & -1 & -1 & 0 \\ -1 & -1 & 0 & -1 & -1 & -1 & 0 & -1 & -1 & -1 & z & 0 & 0 \\ -1 & -1 & -1 & 0 & -1 & -1 & -1 & 0 & -1 & -1 & 0 & z & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{vmatrix}$$

This determinant is equal to the determinant of the first 12 rows and columns. Now, subtract row 5 from row 1, row 6 from row 2, row 7 from row 3, and row 8 from row 4. Then, add column 1 to column 5, column 2 to column 6, column 3 to column 7, and column 4 to column 8 to get

$$(-x+4)\begin{vmatrix} J_4-I_4-xI_4 & \mathbf{0}_{4\times 4} & \mathbf{0}_{4\times 4} \\ \mathbf{0}_{4\times 4} & J_4-I_4-xI_4 & I_4 \\ \mathbf{0}_{4\times 4} & -2J_4+2I_4 & (\bigoplus_2 J_2-I_2)-xI_4 \end{vmatrix}$$

$$= (-x+4)(x-3)(x+1)^3 \begin{vmatrix} J_4 - I_4 - xI_4 & I_4 \\ -2J_4 + 2I_4 & (\bigoplus_2 J_2 - I_2) - xI_4 \end{vmatrix}$$

The last determinant is equal to

$$\begin{vmatrix} -x & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & -x & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & -x & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & -x & 0 & 0 & 0 & 1 \\ 0 & -2 & -2 & -2 & z & 0 & -1 & -1 \\ -2 & 0 & -2 & -2 & 0 & z & -1 & -1 \\ -2 & -2 & 0 & -2 & -1 & -1 & z & 0 \\ -2 & -2 & -2 & 0 & -1 & -1 & 0 & z \end{vmatrix}$$

Now, add 2 times row 1 to row 5, 2 times row 2 to row 6, two times row 3 to row 7, and two times row 4 to row 8, and set $y := -x+1$

$$= \begin{vmatrix} -x & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & -x & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & -x & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & -x & 0 & 0 & 0 & 1 \\ -2x & 0 & 0 & 0 & y & 0 & -1 & -1 \\ 0 & -2x & 0 & 0 & 0 & y & -1 & -1 \\ 0 & 0 & -2x & 0 & -1 & -1 & y & 0 \\ 0 & 0 & 0 & -2x & -1 & -1 & 0 & y \end{vmatrix}$$

$$= \begin{vmatrix} J_4 - (x+1)I_4 & I_4 \\ -2xI_4 & D \end{vmatrix} \tag{3.10}$$

Since D is a regular symmetric matrix, it commutes with J_4 and so, the determinant in (3.10) is equal to $\det[(J_4 - (x+1)I_4)D - 2xI_4]$, which is equal to

$$\begin{vmatrix} x(x+1)-2 & -x-1 & 0 & 0 \\ -x-1 & x(x+1)-2 & 0 & 0 \\ 0 & 0 & x(x+1)-2 & -x-1 \\ 0 & 0 & -x-1 & x(x+1)-2 \end{vmatrix} = \begin{vmatrix} a & b & 0 & 0 \\ b & a & 0 & 0 \\ 0 & 0 & a & b \\ 0 & 0 & b & a \end{vmatrix}$$

and that equals $(a-b)^2(a+b)^2$. So, the determinant (3.10) is equal to

$$(x^2+2x-1)^2(x^2-3)^2$$

and therefore the determinant (3.8), which is the characteristic polynomial of G_2, equals $(x-4)(x-3)(x+1)^3(x^2-3)^2(x^2+2x-1)^2$. So, $\mathcal{E}(G_2) = 10+4(\sqrt{2}+\sqrt{3})$ and thus G_2 is not hyper-energetic.

However, the method used in Example 3.3 will be using in the next section to introduce a class of hyper-energetic graphs.

3.3.1 Generalization and Main Result

Here we introduce a class of graphs with the locally strongly regular property. In fact, the first graph of this class, that we call G_m, is G_2 in Example 3.3.

G_m is a graph with $n = (2m-1)2m+1$ vertices with the following construction:

Consider $2m-2$ copies of K_{2m} and m copies of K_2 and one copy of K_1. Label the graph such that the vertex K_1 is labeled as u_n, the vertices of the m copies of K_2 by $u_1, u_2, \ldots, u_{2m}$, and the vertices of i^{th} copy of K_{2m} as $v_{i1}, v_{i2}, \ldots, v_{i(2m)}$. Add edges to make it $2m$-regular by adding $2m$ edges from u_n to $u_1, u_2, \ldots, u_{2m}$ and join v_{ij} to u_j for $1 \leq i \leq 2m-2$ and $1 \leq j \leq 2m$.

Vertex u_n is the vertex with strongly regular property and has 1 common neighbor with every other vertices of G_m. Therefore, G_m is an LSR graph with parameters $((2m-1)2m+1, 2m, 1)$.

The adjacency matrix of G_m is of order $(2m-1)(2m)+1$ and it is

$$A(G_m) = \begin{bmatrix} J_{2m}-I_{2m} & \mathbf{0}_{2m\times 2m} & \cdots & \mathbf{0}_{2m\times 2m} & I_{2m} & \mathbf{0}_{2m\times 1} \\ \mathbf{0}_{2m\times 2m} & J_{2m}-I_{2m} & \cdots & \vdots & I_{2m} & \mathbf{0}_{2m\times 1} \\ \vdots & \vdots & \ddots & \mathbf{0}_{2m\times 2m} & \vdots & \vdots \\ \mathbf{0}_{2m\times 2m} & \cdots & \mathbf{0}_{2m\times 2m} & J_{2m}-I_{2m} & I_{2m} & \mathbf{0}_{2m\times 1} \\ I_{2m} & I_{2m} & \cdots & I_{2m} & B_{2m\times 2m} & \mathbf{1}_{2m\times 1} \\ \mathbf{0}_{1\times 2m} & \mathbf{0}_{1\times 2m} & \cdots & \mathbf{0}_{1\times 2m} & \mathbf{1}_{1\times 2m} & 0 \end{bmatrix}$$

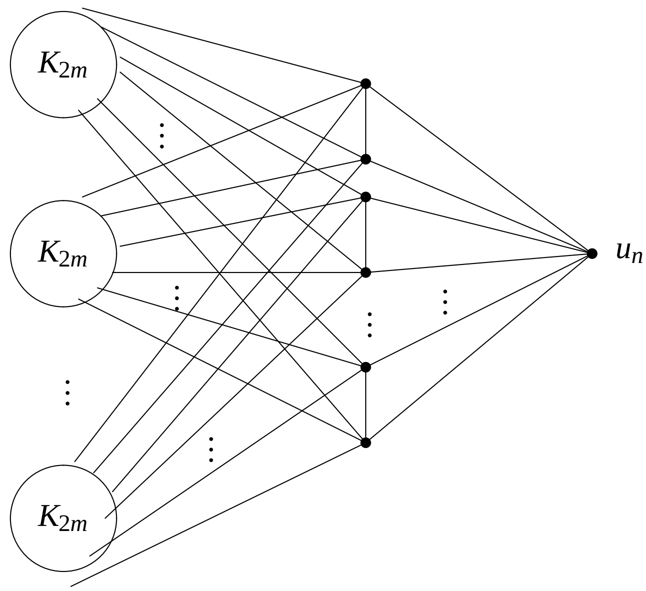


Figure 3.4: An example of local strongly regular graphs

where $B_{2m\times 2m}$ is $\bigoplus_m (J_2 - I_2)$.

In the following, we find the characteristic polynomial of $A(G_m)$ and show that it is equal to

$$(x-2m)(x-(2m-1))^{2m-3}(x+1)^{(2m-3)(2m-1)}$$
$$(x^2-(2m-1))^m(x^2+2x-(2m-3))^m \ .$$

For the simplicity, for matrices $\mathbf{0}_{2m\times 1}$ and $\mathbf{0}_{1\times 2m}$ we just write $\mathbf{0}$ and for matrices $\mathbf{1}_{2m\times 1}$ and $\mathbf{1}_{1\times 2m}$ we just write $\mathbf{1}$. Also, $B = \bigoplus_m (J_2 - I_2)$.

Now, the determinant of $A(G_m) - xI$ equals

$$\begin{vmatrix} J_{2m}-(x+1)I_{2m} & \mathbf{0}_{2m\times 2m} & \cdots & \mathbf{0}_{2m\times 2m} & I_{2m} & \mathbf{0} \\ \mathbf{0}_{2m\times 2m} & J_{2m}-(x+1)I_{2m} & \cdots & \vdots & I_{2m} & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathbf{0}_{2m\times 2m} & \mathbf{0}_{2m\times 2m} & \cdots & J_{2m}-(x+1)I_{2m} & I_{2m} & \mathbf{0} \\ I_{2m} & I_{2m} & \cdots & I_{2m} & B-xI_{2m} & \mathbf{1} \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{1} & -x \end{vmatrix}$$

By adding the first $(2m-1)(2m)$ rows to the last row, extracting the factor $(-x+2m)$ from the determinant; then subtracting the last column from all the other columns and then subtracting the last row from rows $2m(2m-2)+1, \cdots, 2m(2m-1)$, the determinant remains unchanged and it equals:

$$(-x+2m)\begin{vmatrix} J_{2m}-(x+1)I_{2m} & \mathbf{0}_{2m\times 2m} & \cdots & \mathbf{0}_{2m\times 2m} & I_{2m} & \mathbf{0} \\ \mathbf{0}_{2m\times 2m} & J_{2m}-(x+1)I_{2m} & \cdots & \vdots & I_{2m} & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathbf{0}_{2m\times 2m} & \mathbf{0}_{2m\times 2m} & \cdots & J_{2m}-(x+1)I_{2m} & I_{2m} & \mathbf{0} \\ -J_{2m}+I_{2m} & -J_{2m}+I_{2m} & \cdots & -J_{2m}+I_{2m} & B-xI_{2m}-J_{2m} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & 1 \end{vmatrix}$$

$$
= (-x+2m)\begin{vmatrix} J_{2m}-(x+1)I_{2m} & \mathbf{0}_{2m\times 2m} & \cdots & \mathbf{0}_{2m\times 2m} & I_{2m} \\ \mathbf{0}_{2m\times 2m} & J_{2m}-(x+1)I_{2m} & \cdots & \vdots & I_{2m} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0}_{2m\times 2m} & \mathbf{0}_{2m\times 2m} & \cdots & J_{2m}-(x+1)I_{2m} & I_{2m} \\ -J_{2m}+I_{2m} & -J_{2m}+I_{2m} & \cdots & -J_{2m}+I_{2m} & B-xI_{2m}-J_{2m} \end{vmatrix}
$$

If we subtract the block row $[\mathbf{0}_{2m\times 2m}\ \mathbf{0}_{2m\times 2m} \cdots J_{2m}-(x+1)I_{2m}\ I_{2m}]$ from all the blocks above it, and then add the first $2m-3$ block columns to the $(2m-2)$th block column, we get the following

$$
(-x+2m)\begin{vmatrix} J_{2m}-(x+1)I_{2m} & \mathbf{0}_{2m\times 2m} & \cdots & \mathbf{0}_{2m\times 2m} & \mathbf{0}_{2m\times 2m} \\ \mathbf{0}_{2m\times 2m} & J_{2m}-(x+1)I_{2m} & \cdots & \vdots & \mathbf{0}_{2m\times 2m} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0}_{2m\times 2m} & \mathbf{0}_{2m\times 2m} & \cdots & J_{2m}-(x+1)I_{2m} & I_{2m} \\ -J_{2m}+I_{2m} & -J_{2m}+I_{2m} & \cdots & (2m-2)(-J_{2m}+I_{2m}) & B-xI_{2m}-J_{2m} \end{vmatrix}
$$

Add $\dfrac{-1}{2m-2}$ times the $(2m-2)$th block column to all the first $2m-3$ block columns; then add $\dfrac{1}{2m-2}$ times the first $2m-3$ block rows to the

$(2m-2)$th block row to get

$$(-x+2m)\begin{vmatrix} J_{2m}-(x+1)I_{2m} & \mathbf{0}_{2m\times 2m} & \cdots & \mathbf{0}_{2m\times 2m} & \mathbf{0}_{2m\times 2m} \\ \mathbf{0}_{2m\times 2m} & J_{2m}-(x+1)I_{2m} & \cdots & \vdots & \mathbf{0}_{2m\times 2m} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0}_{2m\times 2m} & \mathbf{0}_{2m\times 2m} & \cdots & J_{2m}-(x+1)I_{2m} & I_{2m} \\ \mathbf{0}_{2m\times 2m} & \mathbf{0}_{2m\times 2m} & \cdots & (2m-2)(-J_{2m}+I_{2m}) & B-xI_{2m}-J_{2m} \end{vmatrix}$$

which is equal to

$$(-x+2m)\,|J_{2m}-(x+1)I_{2m}|^{2m-3}\begin{vmatrix} J_{2m}-(x+1)I_{2m} & I_{2m} \\ (2m-2)(-J_{2m}+I_{2m}) & B-xI_{2m}-J_{2m} \end{vmatrix}$$

$$=(-x+2m)(x-(2m-1))^{2m-3}(x+1)^{(2m-3)(2m-1)}|C|$$

where

$$C=\begin{bmatrix} J_{2m}-(x+1)I_{2m} & I_{2m} \\ (2m-2)(-J_{2m}+I_{2m}) & B-xI_{2m}-J_{2m} \end{bmatrix}$$

Now, we just need to compute $|C|$ which equals

$$\begin{vmatrix} J_{2m}-(x+1)I_{2m} & I_{2m} \\ -(2m-2)xI_{2m} & B+(2m-2-x)I_{2m}-J_{2m} \end{vmatrix}. \qquad (3.11)$$

Note that $B+(2m-2-x)I_{2m}-J_{2m}$ is a regular symmetric matrix. Therefore, it commutes with $J_{2m}-(x+1)I_{2m}$. Consequently, by using the formula for the determinant of block matrices, the determinant (3.11) which is equal

$$\det\left[(J_{2m}-(x+1)I_{2m})(B+(2m-2-x)I_{2m}-J_{2m})+(2m-2)xI_{2m}\right]$$

Which is equal to

$$\det\left[(x^2+x-(2m-2))I_{2m}-(x+1)B\right] \tag{3.12}$$

If we set $a := x(x+1)-(2m-2)$ and $b := -x-1$, and rewrite the determinant (3.12), we get

$$\begin{vmatrix} a & b & 0 & 0 & \cdots & \cdots & 0 \\ b & a & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & a & b & \cdots & \cdots & \vdots \\ 0 & 0 & b & a & \cdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & a & b \\ 0 & 0 & \cdots & \cdots & \cdots & b & a \end{vmatrix} = (a-b)^m(a+b)^m$$

Thus, the characteristic polynomial of G_m is

$$(-x+2m)(x-(2m-1))^{2m-3}(x+1)^{(2m-3)(2m-1)}$$
$$(x^2-(2m-1))^m(x^2+2x-(2m-3))^m\ .$$

Theorem 17 *For $m > 2$, graph G_m is hyper-energetic.*

PROOF. For the case $m = 2$, from Example 3.3, it follows that

$$\mathcal{E}(G_2) = 10 + 4(\sqrt{2} + \sqrt{3}) \approx 22.58 < 24$$

and so, G_2 is not hyper-energetic. For $m \geq 3$, we need to show that $\mathcal{E}(G_m)$ is greater than $4m(2m-1)$. If $m = 3$, then $\mathcal{E}(G_m) = 48 + 6\sqrt{5} \approx 61.4164079 > 60$.

For $m \geq 4$ we have $\sqrt{2m-1} + \sqrt{2m-2} > 5$. Therefore,

$$\mathcal{E}(G_m) = 8m^2 - 14m + 2m(\sqrt{2m-1} + \sqrt{2m-2}) + 6$$

$$> 8m^2 - 14m + 10m + 6 = 8m^2 - 4m + 6$$

$$> 8m^2 - 4m = 4m(2m-1)$$

which shows that these graphs are hyper-energetic for $m > 2$. $\square$

Chapter 4

Energy of Digraphs

4.1 Introduction

Peña and Rada in [19] extended the concept of energy for the case of digraphs.

Definition 4.1.1 The energy of a digraph $\mathcal{G}$ with n vertices is defined as

$$\mathcal{E}(\mathcal{G}) = \sum_{i=1}^{n} |Re(\zeta_i)|$$

where $\zeta_1, \ldots, \zeta_n$ are eigenvalues of $\mathcal{G}$.

In fact, it will be proved in Theorem 20, by defining the energy for digraphs in this way that the Coulsons integral formula remains valid. Let $\mathcal{A}$ be the adjacency matrix of a digraph $\mathcal{G}$. The coefficients of the characteristic polynomial $\mathcal{G}$ can be determined as follows.

4.2 Coefficients Theorem

Let $\Phi_{\mathcal{G}}(x) = x^n + b_{n-1}x^{n-1} + \cdots + b_0$ be the characteristic polynomial of digraph $\mathcal{G}$, then the values of b_i's can be found if all the directed cycles of $\mathcal{G}$ are known.

Theorem 18 [5] (Coefficients Theorem for Digraphs) *Let $\mathcal{G}$ be a digraph* *with n vertices. Let $\mathcal{A} = [a_{ij}]$ be its adjacency matrix and*

$$\Phi_{\mathcal{G}}(x) = \det(xI - \mathcal{A}) = x^n + b_{n-1}x^{n-1} + \cdots + b_0$$

be its characteristic polynomial. Then

$$b_{n-i} = \sum_{L \in \mathcal{L}_i} (-1)^{c(L)} \qquad (i = 1, \cdots, n) \tag{4.1}$$

where $\mathcal{L}_i$ is the set of all linear directed subgraphs L (i.e. subgraphs L in which every vertex has indegree and outdegree equal to 1) of G with i vertices, and $c(L)$ is the number of cycles of which L is composed.

PROOF. First, consider $b_0 = \Phi_{\mathcal{G}}(0) = \det(-\mathcal{A}) = (-1)^n \det(\mathcal{A})$. By Leibnitz definition of determinant

$$\det(\mathcal{A}) = \sum_{\sigma \in S_n} (-1)^{N(\sigma)} \prod_{i=1}^{n} a_{i,\sigma(i)}$$

where S_n is the permutation group of order n and $N(\sigma)$ is the parity of the permutation σ. Therefore,

$$b_0 = \sum_{\sigma \in S_n} (-1)^{n+N(\sigma)} a_{1,\sigma(1)} a_{2,\sigma(2)} \cdots a_{n,\sigma(n)}. \tag{4.2}$$

But $(-1)^{n+N(\sigma)} a_{1,\sigma(1)} a_{2,\sigma(2)} \cdots a_{n,\sigma(n)}$ is nonzero if and only if all of the arcs $(1,\sigma(1))$, $(2,\sigma(2))$, $\cdots$, $(n,\sigma(n))$ are in $\mathcal{G}$. Now, σ can be presented as

$$(1\ \sigma(1)\ \ldots)(\ldots)\ldots(\ldots)$$

where parentheses are disjoint in σ. If a term in the sum (4.2) is nonzero, then to each parenthesis in σ there corresponds a cycle in G, therefore, to σ there corresponds a direct sum of disjoint cycles containing n vertices (all vertices) of G, means a linear directed subgraph $L \in \mathcal{L}_n$. On the other hand, a linear directed subgraph L is the union of cycles in G and we could assign a permutation σ to it with the sign depending on the number of cycles of L. So, the theorem is true for b_0.

Suppose $1 \le i < n$ is fixed. It is well-known (for the proof see [3], p.68) that $(-1)^{n-i}b_{n-i}$ is the sum of all principal minors of order $n-i$ of $\mathcal{A}$. Note that the set of these minors is in one-to-one correspondence to the set of induced subgraphs of $\mathcal{G}$ having exactly $n-i$ vertices. Now, the theorem follows by applying the above result to each of the $\binom{n}{i}$ minors, and adding them up. $\square$

An *acyclic* digraph is a digraph containing no directed cycles. By the argument made in Theorem 18, we see that the energy of acyclic digraphs are 0.

EXAMPLE.[19] Consider the digraph $\mathcal{C}_n$ to be the cycle of n vertices (as shown in Figure 4.1).

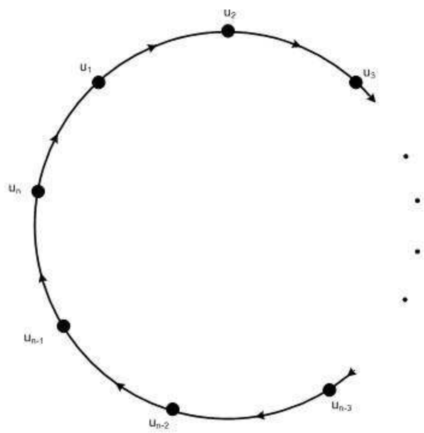


Figure 4.1: Digraph.

Using Theorem 18, the characteristic polynomial of $\mathcal{C}_n$ is $x^n - 1$, and

$$\mathcal{E}\left(\mathcal{C}_n\right) = \sum_{k=0}^{n-1} \left| \cos\left(\frac{2k\pi}{n}\right) \right| \tag{4.3}$$

Similarly, let $\mathcal{G}$ be a digraph with n vertices and a unique cycle $\mathcal{C}_t$ of length t, where $2 \leq t \leq n$. Then

$$\mathcal{E}\left(\mathcal{G}\right) = \mathcal{E}\left(\mathcal{C}_t\right) = \sum_{k=0}^{t-1} \left| \cos\left(\frac{2k\pi}{t}\right) \right| \tag{4.4}$$

Theorem 19 [*19*] *Among all digraphs with n vertices and a unique cycle $\mathcal{C}_t$, the minimal energy is attained when $t = 2, 3,$ or 4 and maximal energy is attained when $t = n$.*

PROOF. Let $\mathcal{G}$ be a digraph with n vertices and a unique cycle $\mathcal{C}_t$ of length $t \geq 2$. Using (4.4), if $t = 2, 3,$ or 4, $\mathcal{E}\left(\mathcal{C}_t\right) = 2$. To complete the first part, we prove that if $t \geq 5$, $\mathcal{E}(\mathcal{C}_t) > 2$. Note that

$$\sum_{r=0}^{t-1} \cos\left(\frac{2r\pi}{t}\right) = 0 \tag{4.5}$$

Therefore,

$$1 + \cos\left(\frac{2\pi}{t}\right) + \sum_{r=2}^{t-1} \cos\left(\frac{2r\pi}{t}\right) = 0$$

So,

$$1 + \cos\left(\frac{2\pi}{t}\right) = -\sum_{r=2}^{t-1} \cos\left(\frac{2r\pi}{t}\right) \leq \sum_{r=2}^{t-1} \left|\cos\left(\frac{2r\pi}{t}\right)\right|$$

Now, since $t > 4$, $\cos(\frac{2\pi}{t}) > 0$, and

$$\mathcal{E}(\mathcal{C}_t) = \sum_{r=0}^{t-1} \left|\cos\left(\frac{2r\pi}{t}\right)\right| = 1 + \cos\left(\frac{2\pi}{t}\right) + \sum_{r=2}^{t-1} \left|\cos\left(\frac{2r\pi}{t}\right)\right|$$

$$\geq 2\left(1 + \cos\left(\frac{2\pi}{t}\right)\right) > 2\ .$$

Next, we prove that for $5 \leq t < n$:

$$\mathcal{E}(\mathcal{C}_t) < \mathcal{E}(\mathcal{C}_n)\ .$$

If $r = 1, \ldots, \lfloor \frac{t}{4} \rfloor$, then $\frac{2r\pi}{n}, \frac{2r\pi}{t} \in (0, \frac{\pi}{2}]$ and since $t < n$, $\cos(\frac{2r\pi}{t}) < \cos(\frac{2r\pi}{n})$.

Now,

$$\mathcal{E}(\mathcal{C}_t) = \sum_{r=0}^{t-1} \left|\cos\left(\frac{2r\pi}{t}\right)\right| = 1 + 2\sum_{r=1}^{\lfloor \frac{t}{4} \rfloor} \cos\left(\frac{2r\pi}{t}\right) - 2\sum_{1+\lfloor \frac{t}{4} \rfloor}^{\lfloor \frac{t}{2} \rfloor} \cos\left(\frac{2r\pi}{t}\right)$$

$$= 1 + 4\sum_{r=1}^{\lfloor \frac{t}{4} \rfloor} \cos\left(\frac{2r\pi}{t}\right) \qquad \text{(by using (4.5))}$$

$$< 1 + 4\sum_{r=1}^{\lfloor \frac{t}{4} \rfloor} \cos\left(\frac{2r\pi}{n}\right) \leq 1 + 4\sum_{r=1}^{\lfloor \frac{n}{4} \rfloor} \cos\left(\frac{2r\pi}{n}\right) = \mathcal{E}\left(\mathcal{C}_n\right).$$

□

4.3 Integral representation of the energy

In this section, we include the proof of Coulson Integral Formula for digraphs given by Peña and Rada in [19].

Theorem 20 [*19*] (Integral representation of the energy) *Let $\mathcal{G}$ be a digraph with n vertices and eigenvalues $\zeta_1, \ldots, \zeta_n$. Then*

$$\frac{1}{\pi}\int_{-\infty}^{+\infty}\left(n - \frac{iz\Phi'_{\mathcal{G}}(iz)}{\Phi_{\mathcal{G}}(iz)}\right)dz = \sum_{i=1}^{n}|Re(\zeta_i)|$$

PROOF. Let $\Phi_{\mathcal{G}}(z) = \prod_{i=1}^{\ell}(z-\nu_i)^{n_i}$ be the characteristic polynomial of the digraph G. The eigenvalues $\nu_1, \ldots, \nu_\ell$ are complex possibly non-real numbers and $\sum_{i=1}^{\ell} n_i = n$.

Now, we have

$$\frac{\Phi'_{\mathcal{G}}(z)}{\Phi_{\mathcal{G}}(z)} = \frac{\sum_{i=1}^{\ell}\left(n_i(z-\nu_i)^{n_i-1}\prod_{j\neq i}(z-\nu_j)^{n_j}\right)}{\prod_{i=1}^{\ell}(z-\nu_i)^{n_i}} = \sum_{i=1}^{\ell}\frac{n_i}{z-\nu_i}$$

Therefore, $\Phi'_{\mathcal{G}}(z)/\Phi_{\mathcal{G}}(z)$ is an analytic function with only ℓ simple poles, $\nu_1, \cdots, \nu_\ell$. Suppose for any $1 \leq k \leq \ell$, we have $\|\nu_k\| \leq \|\nu_1\|$. Choose $r \geq$

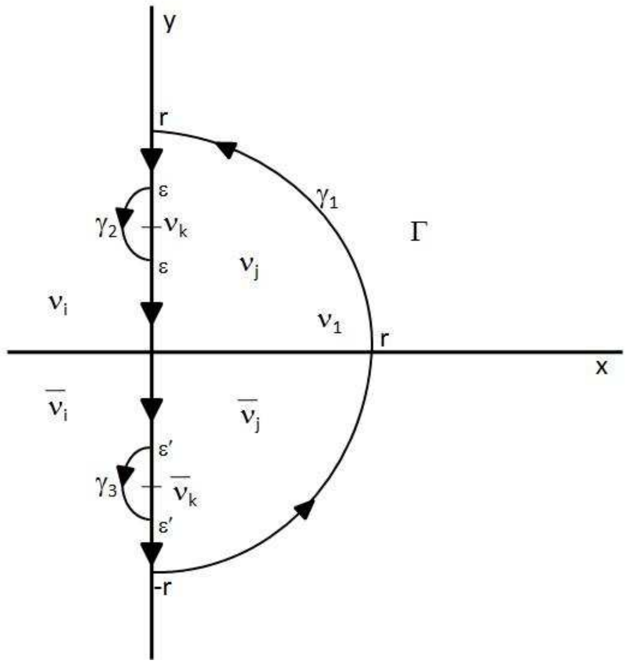


Figure 4.2: Contour Γ

$\|\nu_1\|$. Let Γ be the contour that goes along the y-axis from the point $(0,r)$ to point $(0,-r)$ and returns to $(0,r)$ through a semicircle with radius r. But some of the eigenvalues might appear on the imaginary axis and it is not possible to integrate along a curve passing through a singularity. Note that the coefficients of $\Phi_{\mathcal{G}}(z)$ are real numbers and so, if ν_j is an eigenvalue, its complex conjugate, $\bar{\nu}_j$, is also an eigenvalue. Therefore, we adjust the contour Γ to the one shown in Figure 4.2. Note that only the ν_i's with positive real part are interior to the contour Γ.

Define the function

$$f(z) := z\frac{\Phi'_{\mathcal{G}}(z)}{\Phi_{\mathcal{G}}(z)} = \sum_{i=1}^{\ell} \frac{n_i z}{z-\nu_i}$$

and apply the Cauchy integral formula to it. Now, we have

$$\frac{1}{2\pi i}\oint_{\Gamma} f(z)dz = \frac{1}{2\pi i}\oint_{\Gamma}\sum_{i=1}^{\ell}\frac{n_i z}{z-\nu_i}dz = \frac{1}{2\pi i}\sum_{i=1}^{\ell}\oint_{\Gamma}\frac{n_i z}{z-\nu_i}dz$$

$$= \sum_{+} n_i\nu_i = \sum_{+}\zeta_i = \sum_{+} Re(\zeta_i) = \frac{1}{2}\mathcal{E}(\mathcal{G})$$

where $\sum_{+}$ is taken over the eigenvalues with positive real part. Since n is constant,

$$\frac{1}{2\pi i}\oint_{\Gamma} f(z)dz = \frac{1}{2\pi i}\oint_{\Gamma}[f(z)-n]dz$$

If $\varepsilon \to 0$, we have

$$\int_{\gamma_2}[f(z)-n]dz = -\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}[f(\varepsilon e^{it}+\nu_k)-n]i\varepsilon e^{it}dt = 0$$

Also, if $\varepsilon' \to 0$, we have

$$\int_{\gamma_3}[f(z)-n]dz = -\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}[f(\varepsilon' e^{it}+\overline{\nu_k})-n]i\varepsilon' e^{it}dt = 0$$

On the other hand, since $\sum_{j=1}^{\ell} n_j = n$ we have

$$\int_{\gamma_1}[f(z)-n]dz = \int_{\gamma_1}\sum_{j=1}^{\ell}[\frac{n_j z}{z-\nu_j}-n_j]dz = \int_{\gamma_1}\sum_{j=1}^{\ell}\frac{n_j\nu_j}{z-\nu_j}dz$$

$$= \sum_{j=1}^{\ell} n_j\nu_j\int_{\gamma_1}\frac{1}{z-\nu_j}dz = \sum_{j=1}^{\ell} n_j\nu_j\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{ire^{it}}{re^{it}-\nu_j}dt$$

$$\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{ire^{it}}{re^{it}-\nu_j}dt = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} idt + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{i\nu_j}{re^{it}-\nu_j}dt = \pi i + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{i\nu_j}{re^{it}-\nu_j}dt$$

If $r \to +\infty$, we have $\int_{\gamma_1} \frac{1}{z-\nu_j} dz = \pi i$ and therefore

$$\int_{\gamma_1} \sum_{j=1}^{\ell} \frac{n_j \nu_j}{z-\nu_j} dz = \pi i \sum_{j=1}^{\ell} n_j \nu_j = 0$$

Thus,

$$\frac{1}{2}\mathcal{E}(\mathcal{G}) = \frac{1}{2\pi i} \oint_{\Gamma} [f(z)-n]dz = \frac{1}{2\pi} \int_{+\infty}^{-\infty} [f(iy)-n]dy$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} [n-f(iy)]dy$$

and the result follows. □

4.4 Upper and lower bounds

In [20] and [21], some lower and upper bounds for the energy of digraphs have been found. We present these results.

4.4.1 Upper bound for the energy of digraphs

Rada in [21], found an upper bound for the energy of digraphs in terms of the number of vertices, the number of arcs, and the number of closed walks of a digraph.

Let us denote the number of closed walks of length k in a digraph $\mathcal{G}$ by c_k. If A is the adjacency matrix of digraph $\mathcal{G}$, from elementary graph theory we know that the entry (i,j) in A^k gives the number of walks of length k from i to j. Also, if ζ is an eigenvalue of A, ζ^k is an eigenvalue of A^k. Therefore, the number of closed walks of length k is, in fact, equal to the trace of A^k. Thus, if $\mathcal{G}$ is a digraph with eigenvalues $\zeta_1,\cdots,\zeta_n$, $\sum_{i=1}^n \zeta_i^k = c_k$.

Lemma 4.4.1 [*21*] *If $\mathcal{G}$ is a digraph with n vertices and m arcs and $\zeta_1,\cdots,\zeta_n$ are the eigenvalues of $\mathcal{G}$ then*

$$\sum_{i=1}^{n}(\mathrm{Re}(\zeta_i))^2-\sum_{i=1}^{n}(\mathrm{Im}(\zeta_i))^2=c_2$$

$$\sum_{i=1}^{n}(\mathrm{Re}(\zeta_i))^2+\sum_{i=1}^{n}(\mathrm{Im}(\zeta_i))^2\leq m$$

PROOF. By the argument above,

$$c_2=\sum_{i=1}^{n}\zeta_i^2=\sum_{i=1}^{n}(\mathrm{Re}(\zeta_i))^2-\sum_{i=1}^{n}(\mathrm{Im}(\zeta_i))^2+2i\sum_{i=1}^{n}(\mathrm{Re}(\zeta_i))(\mathrm{Im}(\zeta_i))\ .$$

The first relation follows from the fact that c_2 is an integer.

For the second relation, suppose $A=[a_{ij}]$ is the adjacency matrix of $\mathcal{G}$. Theorem 3 shows that A is unitarily similar to an upper triangular matrix $T=[t_{ij}]$, with $t_{ii}=\zeta_i$. Therefore, $\sum_{i=1}^n\sum_{j=1}^n a_{ij}^2=\sum_{i=1}^n\sum_{j=1}^n|t_{ij}|^2$. By using the fact that A is a $(0,1)$ matrix, we have

$$\sum_{i=1}^{n}(\mathrm{Re}(\zeta_i))^2+\sum_{i=1}^{n}(\mathrm{Im}(\zeta_i))^2=\sum_{i=1}^{n}[(\mathrm{Re}(\zeta_i))^2+(\mathrm{Im}(\zeta_i))^2]=\sum_{i=1}^{n}|\zeta_i|^2=\sum_{i=1}^{n}|t_{ii}|^2$$

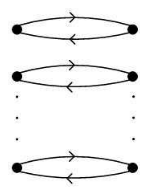
$$\leq \sum_{i=1}^{n}\sum_{j=1}^{n}|t_{ij}|^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}a_{ij}^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}a_{ij} = m$$

$\square$

Theorem 21 [21] *Let $\mathcal{G}$ be a digraph of order n with m edges. Then*

$$\mathcal{E}(\mathcal{G}) \leq \sqrt{\frac{1}{2}n(m+c_2)}$$

where equality holds if and only if $\mathcal{G}$ is a digraph with $\frac{n}{2}$ copies of directed cycle of length 2.



PROOF. We can see that if $\mathcal{G}$ is a digraph with $\frac{n}{2}$ copies of directed cycle of length 2, the eigenvalues of $\mathcal{G}$ consist of $\{1,-1\}$, each with multiplicity $\frac{n}{2}$, and so, $\mathcal{E}(\mathcal{G}) = n = \sqrt{\frac{1}{2}n(n+n)}$. By Lemma 4.4.1 we see that

$$\sum_{i=1}^{n}(\mathrm{Re}(\zeta_i))^2 = \sum_{i=1}^{n}(\mathrm{Im}(\zeta_i))^2 + c_2$$

$$\Rightarrow \quad 2\sum_{i=1}^{n}(\mathrm{Im}(\zeta_i))^2 + c_2 \leq m \quad \Rightarrow \quad \sum_{i=1}^{n}(\mathrm{Im}(\zeta_i))^2 \leq \frac{1}{2}(m-c_2)$$

Suppose $\zeta_1,\cdots,\zeta_n$ are eigenvalues of $\mathcal{G}$. Apply Cauchy-Schwartz inequality to the vectors $(|\mathrm{Re}(\zeta_1)|,\ldots,|\mathrm{Re}(\zeta_n)|)$ and $(1,1,\ldots,1)$

$$\mathcal{E}(\mathcal{G}) = \sum_{i=1}^{n} |\mathrm{Re}(\zeta_i)| \leq \sqrt{n(\sum_{i=1}^{n} (\mathrm{Re}(\zeta_i))^2)} = \sqrt{n(\sum_{i=1}^{n} (\mathrm{Im}(\zeta_i))^2 + c_2)}$$

$$\leq \sqrt{n(\frac{1}{2}(m - c_2) + c_2)} = \sqrt{\frac{1}{2}n(m + c_2)} \tag{4.6}$$

We remain to prove that if the equality happens then $\mathcal{G}$ is a digraph with $\frac{n}{2}$ copies of directed cycle of length 2. Suppose $\mathcal{E}(\mathcal{G}) = \sqrt{\frac{1}{2}n(m + c_2)}$. Since the isolated vertices do not change the energy, we can assume that $\mathcal{G}$ has no isolated vertices. On the other hand, with this assumption, all the inequalities in 4.6 are now equalities and so, $\sum_{i=1}^{n} |\mathrm{Re}(\zeta_i)| = \sqrt{n \sum_{i=1}^{n} (\mathrm{Re}(\zeta_i))^2}$. Therefore, we have

$$\mathrm{Re}(\zeta_1) = \mathrm{Re}(\zeta_2) = \ldots = \mathrm{Re}(\zeta_n) = \ell \in \mathbb{R}\ .$$

Recall from Section 2.2 that the spectral radius r of the adjacency matrix is an eigenvalue of $\mathcal{G}$ and so, $\ell = r$. On the other hand, we have $\ell = |\mathrm{Re}(\zeta_i)| \leq |\zeta_i| \leq r$ and so, $|\mathrm{Re}(\zeta_i)| = |\zeta_i| = r$, $i = 1, \ldots, n$, which implies that all eigenvalues of $\mathcal{G}$ are real with absolute value r. Therefore, $nr = \mathcal{E}(\mathcal{G}) = \sqrt{\frac{1}{2}n(m + c_2)}$ and $c_2 = \sum_{i=1}^{n} \zeta_i^2 = nr^2$. Combining two relations, we have

$$nr = \sqrt{\frac{1}{2}n(m + nr^2)} \ \Rightarrow\ nr^2 = m \ \Rightarrow\ c_2 = m$$

which means the number of closed walks of length 2 in $\mathcal{G}$ equals the number of arcs of $\mathcal{G}$ and therefore $\mathcal{G}$ is a symmetric digraph with $\mathcal{E}(\mathcal{G}) = \sqrt{nm}$. Recall from page 9 that there is a bijection ψ between graphs and symmetric digraphs. Let G be the graph such that $\psi(G) = \mathcal{G}$. If k is the number of edges in G, $\mathcal{E}(\mathcal{G}) = \mathcal{E}(G) = \sqrt{2nk}$. Note that $\mathcal{G}$ and G have no isolated vertices and so, $2k \geq n$. Using the Cauchy-Schwartz inequality in a similar fashion as it was used in the proof of Theorem 11, together with the equality $\sum_{i=1}^{n} \zeta_i^2 = 2k$, we can see that $\mathcal{E}(G) = \sqrt{2nk}$ if and only if G is $\frac{n}{2}$ copies of K_2. Therefore, $\mathcal{G}$ is $\frac{n}{2}$ copies of directed cycle of length 2. $\square$

A natural question here is to find an upper bound depending only on the number of vertices and arcs, as it was found by Koolen and Moulton for the case of graphs. Suppose $\mathcal{G}$ is a strongly connected digraph with n vertices and m arcs. Recall from Section 2.1 (page 11), that $n \leq m$. By using the fact that $c_2 \leq m$, we have

$$\mathcal{E}(\mathcal{G}) \leq \sqrt{\frac{1}{2}n(m+c_2)} \leq \sqrt{nm} \leq \sqrt{m^2} = m \tag{4.7}$$

If equality happens, then $nm = m^2$, which implies $m = 0$ or $m = n$. If $m = 0$ then $\mathcal{G}$ is a vertex. Otherwise $m = n$, and we also have $\sqrt{\frac{1}{2}n(m+c_2)} = \sqrt{nm}$ which means $c_2 = m = n$.

Rada in [21] proved that the relation $\mathcal{E}(\mathcal{G}) \leq m$ is true for every digraph, and therefore an upper bound in terms of the number of arcs exists for the energy of digraphs. We include here the proof of Rada for the relation (4.7) for every digraphs.

Theorem 22 [*21*] *Let $\mathcal{G}$ be a digraph with m arcs. Then we have*

$$\mathcal{E}(\mathcal{G}) \leq m$$

and the equality holds if and only if $\mathcal{G}$ consists of $\frac{m}{2}$ copies of directed cycle of length 2 *plus some isolated vertices.*

PROOF. As we have seen on (4.7), the statement is true for strongly connected digraphs. Suppose $\mathcal{G}$ has n vertices. Let $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$ be the strongly connected components of $\mathcal{G}$ such that for $i = 1, 2, \ldots, k$, n_i and m_i are the number of vertices and arcs of $\mathcal{C}_i$, respectively. Then,

$$\sum_{i=1}^{k} n_i = n \quad \text{and} \quad \sum_{i=1}^{k} m_i \leq m \, .$$

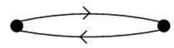
Denote the characteristic polynomial of G by $\Phi_G(x)$. By Theorem 1, we have

$$\Phi_{\mathcal{G}}(x) = \Phi_{\mathcal{C}_1}(x)\Phi_{\mathcal{C}_2}(x)\cdots\Phi_{\mathcal{C}_k}(x)$$

and therefore,

$$\mathcal{E}(\mathcal{G}) = \sum_{i=1}^{k} \mathcal{E}(\mathcal{C}_i) \leq \sum_{i=1}^{k} m_i \leq m \, .$$

For the second part, if $\mathcal{G}$ is a graph consists of $\frac{m}{2}$ directed cycle of length 2 then $\mathcal{E}(\mathcal{G}) = m$. For the converse, if $\mathcal{G}$ is strongly connected digraph, by argument before the theorem, we have $c_2 = m = n$ and so, $\mathcal{G}$ is a directed cycle of length 2.



For the general case, we have

$$\sum_{i=1}^{k} \mathcal{E}(\mathcal{C}_i) = \sum_{i=1}^{k} m_i = m \, .$$

For each i, we have $\mathcal{E}(\mathcal{C}_i) \leq m_i$. Therefore, $\mathcal{E}(\mathcal{C}_i) = m_i$, $i = 1, \ldots, k$ and so, each $\mathcal{C}_i$ is a directed cycle of length 2 or a vertex. $\square$

4.4.2 Lower bound for the energy of digraphs

As we have seen in page 57, the energy of an acyclic digraph is zero. On the other hand, let $\mathcal{G}$ be a digraph with $\mathcal{E}(\mathcal{G}) = 0$. If $\mathcal{G}$ is of order n with eigenvalues $\zeta_1, \ldots, \zeta_n$, then $\operatorname{Re}(\zeta_i) = 0$, $i = 1, \ldots, n$. Let r be the spectral radius of $\mathcal{G}$. Since the adjacency matrix of $\mathcal{G}$ is non-negative, r is real and non-negative and it belongs to the spectrum of $\mathcal{G}$. In particular $r = 0$ and so, $\zeta_i = 0$, $i = 1, \ldots, n$. This shows that $\Phi_{\mathcal{G}}(x) = x^n$ and so, $\mathcal{G}$ is an acyclic digraph. Therefore, the minimal energy 0 is attained in acyclic digraphs.

Rada in [20] found a lower bound for the energy of digraphs in terms of the number of closed walks of a digraph. Here, we include the result of Rada.

Theorem 23 [20] *Let $\mathcal{G}$ be a digraph of order n with eigenvalues $\zeta_1, \ldots, \zeta_n$. If A is the adjacency matrix of $\mathcal{G}$ and c_2 is the number of closed walks of* *length* 2 *in* $\mathcal{G}$, *we have*

$$\mathcal{E}(\mathcal{G}) \geq \sqrt{2c_2} \tag{4.8}$$

and equality holds if and only if $\mathcal{G}$ *is acyclic or the eigenvalues of* $\mathcal{G}$ *are* $0, -\sqrt{c_2/2}, \sqrt{c_2/2}$ *with multiplicities* $n-2, 1, 1$ *respectively.*

PROOF. Since all the diagonal entries in A are 0, $trA = 0$ and we have

$$0 = \left(\sum_{i=1}^{n} \mathrm{Re}(\zeta_i)\right)^2 = \sum_{i=1}^{n} (\mathrm{Re}(\zeta_i))^2 + 2\sum_{i<j} (\mathrm{Re}(\zeta_i))(\mathrm{Re}(\zeta_j)) \tag{4.9}$$

Now, by triangular inequality we have

$$\begin{aligned}
(\mathcal{E}(\mathcal{G}))^2 = \left(\sum_{i=1}^{n} |\mathrm{Re}(\zeta_i)|\right)^2 &= \sum_{i=1}^{n} (\mathrm{Re}(\zeta_i))^2 + 2\sum_{i<j} |\mathrm{Re}(\zeta_i)||\mathrm{Re}(\zeta_j)| \\
&\geq \sum_{i=1}^{n} (\mathrm{Re}(\zeta_i))^2 + 2\left|\sum_{i<j} \mathrm{Re}(\zeta_i)\mathrm{Re}(\zeta_j)\right| \\
&= 2\sum_{i=1}^{n} (\mathrm{Re}(\zeta_i))^2
\end{aligned}$$

On the other hand, by Lemma 4.4.1,

$$c_2 = \sum_{i=1}^{n} (\mathrm{Re}(\zeta_i))^2 - \sum_{i=1}^{n} (\mathrm{Im}(\zeta_i))^2 \leq \sum_{i=1}^{n} (\mathrm{Re}(\zeta_i))^2 \tag{4.10}$$

and the inequality (4.8) is established.

Assume $\mathcal{G}$ is not acyclic and the equality happens in (4.8). Then the equality also holds in (4.10) and so, $\sum_{i=1}^{n} (\mathrm{Im}(\zeta_i))^2 = 0$, which shows that all the eigenvalues of $\mathcal{G}$ are real.

In addition, we have $\sum_{i<j} |\mathrm{Re}(\zeta_i)||\mathrm{Re}(\zeta_j)| = \left|\sum_{i<j} \mathrm{Re}(\zeta_i)\mathrm{Re}(\zeta_j)\right|$, which is possible only when all the ζ_i's have the same sign or all are zero except two of them with opposite signs. By (4.9), we have $\sum_{i<j} \mathrm{Re}(\zeta_i)\mathrm{Re}(\zeta_j) < 0$. Therefore, exactly two of the eigenvalues are nonzero with opposite signs, say $\zeta, -\zeta$. Therefore, the characteristic polynomial of $\mathcal{G}$ is

$$\Phi_{\mathcal{G}}(x) = (x-\zeta)(x+\zeta)x^{n-2} = x^n - \zeta^2 x^{n-2}$$

By Theorem 18, $\zeta = \sqrt{c_2/2}$ and the proof is complete. $\square$

4.5 Energy of some digraphs

In this section we find the energy of some classes of digraphs.

Let q be a prime power such that $q \equiv 3 \pmod 4$. Let S be the set of square elements of the finite field $\mathbb{F}_q^*$. Then $-1 \notin S$, and so, for each pair (a,b) of distinct elements of $\mathbb{F}_q$, either $a-b \in S$ or $b-a \in S$, but not both. Now, we define the *Paley digraph* as the directed graph $\mathcal{P}_q := (\mathcal{V}, A_q)$ with vertices $\mathcal{V} = \mathbb{F}_q$ and arcs $A_q = \{(a,b) \in \mathbb{F}_q \times \mathbb{F}_q \,:\, b-a \in S\}$. (see Figure 4.3)

In the following theorem, we are introducing the relation between the energy of the Paley digraph and the energy of its underlying graph.

Theorem 24 *Let $q \equiv 3 \pmod 4$ be a prime power. The energy of the Paley digraph $\mathcal{P}_q$ of order q is one half of the energy of its underlying graph.*

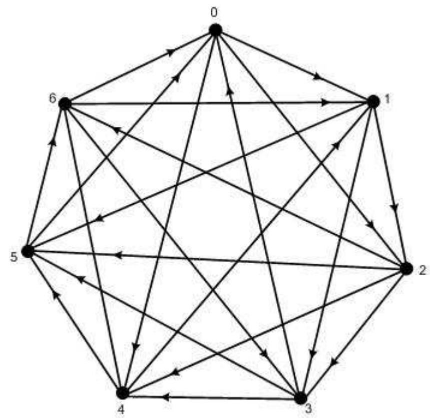


Figure 4.3: $\mathcal{P}_7$: Paley digraph of order 7

PROOF. By the definition of Paley digraph, for indices i, j where $i \neq j$, either $a_{ij} = 1, a_{ji} = 0$ or $a_{ij} = 0, a_{ji} = 1$. Therefore, $A_q + A_q^t = J_q - I_q$, $A_q J_q = J_q A_q$, and $A_q^t J_q = J_q A_q^t$. Now, by using $A_q^t(J_q - I_q) = (J_q - I_q)A_q^t$ we have the following:

$$A_q^t(A_q + A_q^t) = A_q^t(J_q - I_q)$$

$$(A_q + A_q^t)A_q^t = (J_q - I_q)A_q^t = A_q^t(J_q - I_q)$$

$$A_q^t A_q = A_q A_q^t = A_q^t(J_q - I_q) - (A_q^t)^2$$

Therefore A_q and A_q^t commute and so A_q is a normal matrix.*

By Theorem 4, there exists a unitary matrix U of order q in such a way that both $U^* A_q U$ and $U^*(J_q - I_q)U$ are diagonal matrices. Let $U^* A_q U = \mathrm{diag}(\lambda_1, \ldots, \lambda_q)$, then $U^* A_q^t U = \mathrm{diag}(\overline{\lambda_1}, \ldots, \overline{\lambda_q})$, we have $U^*(A_q + A_q^t)U =$

*Note. In fact A_q form a symmetric design ([24]) and obviously A_q and A_q^t commute. Here, we have given the proof not relying on this fact.

$\operatorname{diag}(\lambda_1+\overline{\lambda_1},\ldots,\lambda_q+\overline{\lambda_q}) = U^*(J_q - I_q)U$. Therefore $\{\lambda_i+\overline{\lambda_i} : 1 \le i \le q\}$ is exactly all the eigenvalues of $J_q - I_q$. It follows now that $2\mathcal{E}(\mathcal{P}_q) = \mathcal{E}(K_q)$ $\square$

EXAMPLE. Consider the matrix

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

As described in Theorem 6, for $i = 1,2,3,$ and 4, define C_i by $C_4 = \mathbf{0}_{4\times 4}$ and

$$C_1 = \begin{bmatrix} 1 & - & - & 1 \\ - & 1 & 1 & - \\ - & 1 & 1 & - \\ 1 & - & - & 1 \end{bmatrix}, C_2 = \begin{bmatrix} 1 & - & 1 & - \\ - & 1 & - & 1 \\ 1 & - & 1 & - \\ - & 1 & - & 1 \end{bmatrix}, C_3 = \begin{bmatrix} 1 & 1 & - & - \\ 1 & 1 & - & - \\ - & - & 1 & 1 \\ - & - & 1 & 1 \end{bmatrix}$$

Next consider the following matrix

$$H_{16} = \begin{bmatrix} \mathbf{0} & C_1 & C_2 & C_3 \\ -C_1 & \mathbf{0} & C_3 & C_2 \\ -C_2 & -C_3 & \mathbf{0} & C_1 \\ -C_3 & -C_2 & -C_1 & \mathbf{0} \end{bmatrix}$$

Let D_1 be the matrix derived from H_{16} by changing "1" to "0" and " $-$ " to "1" and D_2 be the matrix derived from H_{16} by changing " $-$ " to "0". Then D_1 and D_2 are adjacency matrices of digraphs $\mathcal{G}_1$ and $\mathcal{G}_2$ shown in Figure 4.4. D_2 is, in fact, the transpose of D_1 and the characteristic polynomials of both D_1 and D_2 are the same and it equals to $(x^2+4)^6(x-6)(x+2)^3$. So, by Definition 4.1.1, the energy of digraphs D_1 and D_2 equals 12. On the other hand, D_1+D_2 is the adjacency matrix for the underlying graph of both $\mathcal{G}_1$ and $\mathcal{G}_2$.

$$D_1+D_2 = \begin{bmatrix} \mathbf{0}_{4\times 4} & \mathbf{1}_{4\times 4} & \mathbf{1}_{4\times 4} & \mathbf{1}_{4\times 4} \\ \mathbf{1}_{4\times 4} & \mathbf{0}_{4\times 4} & \mathbf{1}_{4\times 4} & \mathbf{1}_{4\times 4} \\ \mathbf{1}_{4\times 4} & \mathbf{1}_{4\times 4} & \mathbf{0}_{4\times 4} & \mathbf{1}_{4\times 4} \\ \mathbf{1}_{4\times 4} & \mathbf{1}_{4\times 4} & \mathbf{1}_{4\times 4} & \mathbf{0}_{4\times 4} \end{bmatrix}. \tag{4.11}$$

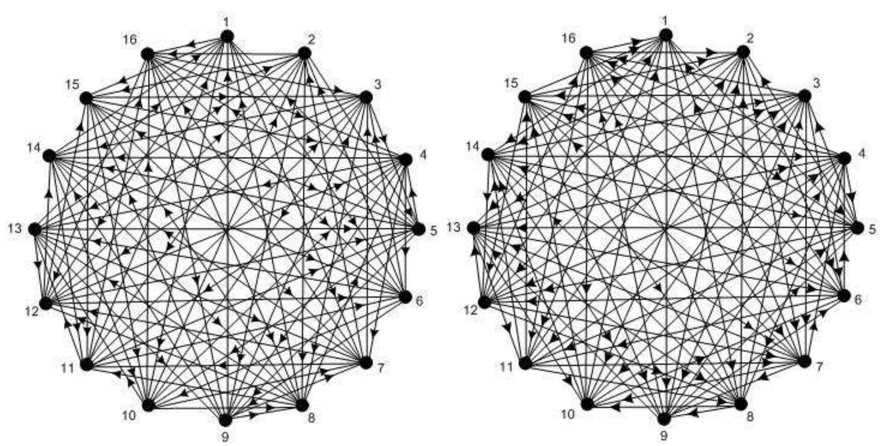


Figure 4.4: Digraphs for matrices D_1 and D_2

The characteristic polynomial of D_1+D_2 is $x^{12}(x-12)(x+4)^3$ and so, the energy of the underlying graph is 24.

In general case, we may use the methods of Theorem 6. Let $H = [\mathbf{c}_1\ \mathbf{c}_2\ \ldots\ \mathbf{c}_n]$ be a Hadamard matrix of order $n = 4m$ where $\mathbf{c}_i$s are columns of H and the last column equals all-one column. Define $C_i = \mathbf{c}_i\mathbf{c}_i^t$, $i = 1, \cdots, n-1$ as it was in the proof of Theorem 6. Now, consider a symmetric Latin square L of order n with numbers $\{1, \cdots, n\}$ and n on the diagonal ([13]). Construct the matrix M by changing each number i above the diagonal of L with C_i and each i below the diagonal of L with $-C_i$ and change the n on the diagonal with a $\mathbf{0}_{n\times n}$ matrix.

Let D_1 be the matrix derived from M by changing 1 to 0 and $-$ to 1, and D_2 be the matrix derived from M by changing $-$ to 0. Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be their corresponding digraphs, respectively. Let $D_3 = D_1 + D_2$ with its corresponding graph G_3, then D_3 is of the form

$$D_3 = D_1 + D_2 = \begin{bmatrix} \mathbf{0}_{4m\times 4m} & \mathbf{1}_{4m\times 4m} & \cdots & \mathbf{1}_{4m\times 4m} \\ \mathbf{1}_{4m\times 4m} & \mathbf{0}_{4m\times 4m} & \cdots & \mathbf{1}_{4m\times 4m} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{1}_{4m\times 4m} & \mathbf{1}_{4m\times 4m} & \cdots & \mathbf{0}_{4m\times 4m} \end{bmatrix}.$$

Theorem 25 *Let $n = 4m$. The energy of the digraph $\mathcal{G}_1$ of order n^2 that we constructed above is one half of the energy of its underlying graph, G_3. Furthermore, $\mathcal{E}(\mathcal{G}_1) = \mathcal{E}(\mathcal{G}_2) = \frac{1}{2}\mathcal{E}(G_3) = n(n-1)$*

PROOF. Since the Latin square L is symmetric, we see that D_2 is the transpose of D_1, i.e. $D_2 = D_1^t$. Note that since D_1 is a real matrix D_1^t and D_1^* are the same.

REMARK. The fact that D_1 and D_1^t commute follows from the observation that D_1 form a symmetric design ([24], [13]). We have opted to give a proof here not relying on this fact.

We have

$$D_1^t(D_1 + D_1^t) = D_1^t D_3 = J_{n(n-1)/2}\ . \tag{4.12}$$

$$(D_1 + D_1^t)D_1^t = D_3 D_1^t = J_{n(n-1)/2}$$

$$D_1^t D_1 = D_1 D_1^t = J_{n(n-1)/2} - (D_1^t)^2$$

Therefore, D_1 and D_1^t commute and so D_1 is normal. From (4.12) we can also see that D_1 and D_3 commute. Now, by Theorem 4, there exists a unitary matrix U of order n^2 in such a way that both U^*D_1U and U^*D_3U are diagonal matrices. Let $U^*D_1U = \mathrm{diag}(\lambda_1, \ldots, \lambda_{n^2})$, then $U^*D_1^tU = \mathrm{diag}(\overline{\lambda_1}, \ldots, \overline{\lambda_{n^2}})$, we have $U^*(D_1 + D_1^t)U = \mathrm{diag}(\lambda_1 + \overline{\lambda_1}, \ldots, \lambda_{n^2} + \overline{\lambda_{n^2}}) = U^*D_3U$. Therefore $\{\lambda_i + \overline{\lambda_i} : 1 \leq i \leq n^2\}$ is exactly all the eigenvalues of D_3. It follows now that $2\mathcal{E}(\mathcal{G}_1) = \mathcal{E}(G_3)$

Now, we need to just compute the energy of G_3. We use the method of equitable partition (Section 2.2). We partition D_3 into the blocks of order $n = 4m$. Let B be the quotient matrix for D_3. Then

$$B = \begin{bmatrix} 0 & n & \cdots & n \\ n & 0 & \cdots & \vdots \\ \vdots & \vdots & \ddots & n \\ n & \cdots & n & 0 \end{bmatrix}$$

and the eigenvalues of B are

$$-n \qquad (\text{with multiplicity } n-1)$$

$$n(n-1) \qquad (\text{with multiplicity } 1)$$

which are also the nonzero eigenvalues of D_3 by Lemma 2.2.2. The rank of D_3 is n, therefore, the other eigenvalues of D_3 are 0. Consequently the energy of G_3 which is in fact the underlying graph of $\mathcal{G}_1$ and $\mathcal{G}_2$ is $2n(n-1)$. Therefore, $\mathcal{E}(\mathcal{G}_1) = \mathcal{E}(\mathcal{G}_2) = n(n-1)$. $\square$

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