Example 2.3.1. Degree matrix of Graph G (b) is

$$\begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

2.1 Laplacian matrix

Definition 2.4.1. Let G be a graph with $V(G) = \{v_1, v_2, ..., v_n\}$ and $E(G) = \{e_1, e_2, ... e_m\}$. The Lapacian matrix of G is the $n \times n$ matrix whose entries $l_{i,j}$ are defined as follows,

$$l_{i,j} = \begin{cases} d_i & \text{if } i = j \\ -1 & v_i \text{ Adjacent } v_j \\ 0 & \text{otherwise} \end{cases}$$

The Laplacian matrix is denoted by L(G).

Example 2.4.1. Consider figure 2.5,

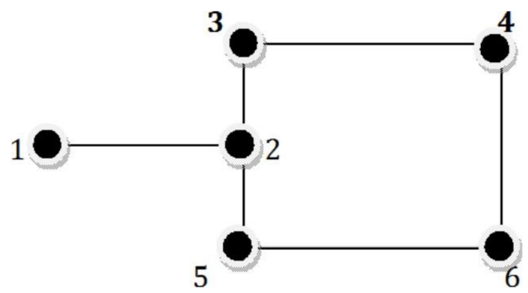

Figure 2.5: A graph with 5 vertices and 6 edges

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

$$\Delta(G) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

$$L(G) = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & 0 & -1 \\ 0 & -1 & 0 & 0 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{bmatrix}$$

- The diagonal entries of $L(G)$ are the degree of the corresesonding vertex and note that $L(G) = \Delta(G) - A(G)$.

- Laplacian matrix is also known as Kirchoff matrix.

Given any orientation to the edges,label the edges. The vertex edge incidence matrix Q.

$$q_{i,j} = \begin{cases} +1 & \text{if } v_i \text{ is the positive end of } e_j \\ -1 & \text{if } v_i \text{ is the negative end of } e_j \\ 0 & \text{otherwise} \end{cases}$$

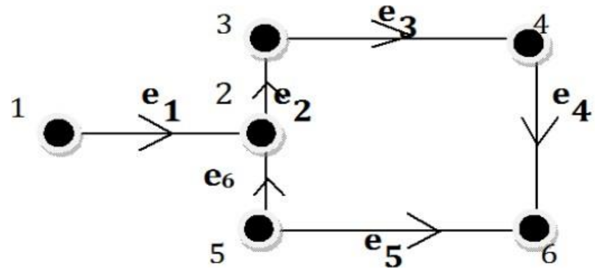

Figure 2.6: Oriented graph with 6 vertices and 6 edges

For this graph we have

$$Q(G) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & -1 & -1 & 0 \end{bmatrix}$$

Then observe that $Q(G).Q(G)^T = L(G)$.

Lemma 2.4.1. Let G be a graph with $V(G) = v_1, v_2, ...v_n$ and $E(G) = e_1, e_2, ...e_n$. Then the following sections hold.

1. L(G) is a symmetric, positive semi definite matrix.
2. The rank of $L(G)$ equals $n - k$, where k is the number of connected components of G
3. For any vector x, $x^r L(G)x = \sum_{i,j} (x_i - x_j)^2$
4. The row sum and column sum of $L(G)$ are zero.

Proof. 1. It is obvious from $L(G) = Q(G).Q(G)^{'}$ that $L(G)$ is symmetric and positive semidefinite. since,

$$\begin{aligned} detL(G) &= detQ(G)detQ(G^{'}) \\ &= detQ(G)detQ(G) \\ &= detQ(G)^2 \\ &\geq 0 \end{aligned}$$

and

$$\begin{aligned} L(G)^T &= (Q(G).Q(G)^{'})^{'} \\ &= (Q(G)^{'})^{'}.Q(G)^{'} \\ &= Q(G)Q(G)^{'} \end{aligned}$$

2. Observe that,

$$rank(G) = (rankQ(G).Q(G)^{'})$$
$$min\{rankQ(G), rankQ(G)^{'}\} = rankQ(G)$$
$$= n - k$$

3. $x^{'}L(G)x = x^{'}Q(G)Q(G)^{'}x$

   The vector $x^{'}Q(G)$ is indexed by the edge $e = \{i, j\}$ is (x_i, x_j).

   Hence $x^{'}Q(G)Q(G)^{'}x = (x_i, x_j)(x_i, x_j) = (x_i, x_j)^2$

4. This follows from the definition $L(G) = \Delta(G) - A(G)$.

□

Chapter 3

The Energy Of Graph

3.1 Energy of graph

The energy E(G) of a graph G is defined to be the sum of the absolute values of Eigen values of G. Hence if A(G) is the adjacency matrix of G and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are Eigen values of A(G) then

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

As the sum of the absolute values of Eigen values . The energy of any graph G, E(G) is always greater than or equal to zero. Since for the totaly disconnected graph K^c_n is the adjacency matrix is a zero matrix. There for it has no nonzero Eigen values. Thus the energy of totally disconnected graph is zero [2] that is $E(K^c_n) = 0$ and thus zero is connected as the lower bound for graph energy.

Example 3.1.1. The complete graph K_n has energy $2(n-1)$.

We have Eigen values of K_n are $n-1$ and $-1, -1, \ldots.. -1\{n-1\ times\}$ There for

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

$$= (n-1) + 1 + 1 + 1 + \ldots\ldots + 1$$

$$= 2(n-1)$$

Result 1. Energy of a disconnected graph is the sum of the energies of its connected.

Proof. Let G be a disconnected graph with n components. Let $G_1, G_2, \qquad G_n$ be its components and let A(G) be the adjacency matrix of G. Construct the vertex set V of G as by considering the vertices of the component G_1 first and followed by the vertices of G_2 and then vertices of G_3 and follow like this and consider the vertices of G_n at last.

If $A(G_1), A(G_2), \ldots\ldots.A(G_n)$ are adjacency matrixes of $G_1, G_2, \ldots\ldots\ldots G_n$ respectively and 0 represents the matrix of all entries zero, then $A(G)$ has the following form

$$A(G) = \begin{bmatrix} A(G_1) & 0 & 0 & \ldots & 0 & 0 \\ 0 & A(G_2) & 0 & \ldots & 0 & 0 \\ . & . & . & . & . & . \\ 0 & 0 & 0 & \ldots & A(G_{n-1}) & 0 \\ 0 & 0 & 0 & \ldots & 0 & A(G_n) \end{bmatrix}$$

Then by a theorem from matrix theory, we have the Eigen values of A(G) is same as the union of the Eigen values of the components $A(G_1), A(G_2), \ldots\ldots A(G_n)$. Let K_j is the order of the component G_j and let $\lambda_{i,1}, \lambda_{i,2}, \ldots\ldots\lambda_{i,n}$(*i.e.*, $\lambda_{i,j}$, $i = 1, 2, \ldots k_j$)are the Eigen values of G are given by,

$\{\lambda_{i,j} : i = 1, 2, 3, \ldots.k_j \text{ and } j = 1, 2, \ldots.n\}$. Thus

$$E(G) = \sum_{I}\sum_{J} |\lambda_{i,j}|$$
$$= \sum_{J} E(G_J)$$

That is $E(G) = E(G_1) + E(G_2) + \ldots\ldots. + E(G_n)$. Thus we can conclude that "the energy of a graph G is same as the sum of the energies of its connected components". □

Result 2. for a simple graph G with Eigen values $\lambda_1, \lambda_2, \ldots\lambda_n$, we have

$$\sum\{\lambda_i : \lambda_i > 0\} = \sum\{\lambda_i \ : \lambda_i < 0\} = \frac{1}{2}E(G)$$

Proof. Let G be a simple graph having n vertices and m edges. Let A(G) be the adjacency matrix of G, and let $\lambda_1, \lambda_2, \ldots\ldots\ldots\lambda_n$ are Eigen values of G. Since the adjacency matrix of a simple graph is symmetric matrix having zeroes on the diagonal. We have sum of its diagonals is again zero.

That is $trace\ A = 0$. But we have ,

$$\sum_{i=1}^{n} \lambda_i = trace\ A$$
$$\Longrightarrow \sum_{i=1}^{n} \lambda_i = 0$$
$$\Longrightarrow \sum\{\lambda_i : \lambda_i > 0\} + \sum\{\lambda_i : \lambda_i < 0\} = 0$$

$$\Longrightarrow \sum \{\lambda_i : \lambda_i > 0\} = -\sum \{\lambda_i : \lambda_i < 0\} \qquad (1)$$

$$
\begin{aligned}
Now \;\; E(G) &= \sum |\lambda_i| \\
&= \sum \{|\lambda_i| : \lambda_i > 0\} + \sum \{|\lambda_i| : \lambda_i < 0\} \\
&= \sum \{\lambda_i : \lambda_i > 0\} - \sum \{\lambda_i : \lambda_i < 0\} \\
&= 2 \sum \{\lambda_i : \lambda_i > 0\}
\end{aligned}
$$

Therefor $\sum \{\lambda_i : \lambda_i > 0\} = \frac{1}{2}E(G)$

Therefore by (1) we can conclude that

$$-\sum \{\lambda_i : \lambda_i < 0\} = \sum \{\lambda_i : \lambda_i > 0\} = \tfrac{1}{2}E(G)$$

In graph theory there is a result that showing bounds of Eigen values of G. "Let λ be an Eigen value of a graph G with n vertices and m edges, then

$$|\lambda_i| \leq \sqrt{\frac{2m(n-1)}{n}}$$

From this we shall obtain the following result. □

Result 3. Let G be a simple graph with n vertices and m edges and having Eigen values $\lambda_1, \lambda_2, \ldots \lambda_n$ then,

$$E(G) \leq \sqrt{2mn(n-1)}$$

Proof. By the above result we have,

$$|\lambda_i| \leq \sqrt{\frac{2m(n-1)}{n}} \qquad \forall \; i = 1, 2, \ldots n$$

Therefore,

$$
\begin{aligned}
E(G) &= \sum_{i=1}^{n} |\lambda_i| \\
&\leq \sum_{i=1}^{n} \sqrt{\frac{2m(n-1)}{n}} \\
&\leq n \times \sqrt{\frac{2m(n-1)}{n}} \\
&= \sqrt{2mn(n-1)}
\end{aligned}
$$

That is, $E(G) \leq \sqrt{2mn(n-1}$ □

3.2 Hyper-energitic and Non-hyper-energitic graph

Since the complete graph Kn, the graph with the maximum possible number of edges (among graph on n vertices) has energy $2(n-1)$. **I.Gutman** (in 1978)conjectured in the paper [6] that "All graphs have energy atmost $2(n-1)$". But then this was disproved by Chris Godsil, by introducing an n vertex graph having energy greater than $2(n-1)$.

Definition 3.2.1. A graph G having energy greater than the energy of the complete graph on the same number of vertices is called a **hyper energetic graph**. That is if for a graph in n vertices $E(G) > 2(n-1)$ then G is called a hyper energetic graph.

Definition 3.2.2. A graph G having energy less than or equal to the energy of the complete graph on the same number of vertices is called **non hyper-**

energetic graph. That is G is an n vertex graph and if $E(G) \leq 2(n-1)$, then G is called a non hyperenergetic graph. A **Circulant matrix** is a special kind of Toeplitz matrix (matrices with constant diagonals are called Toeplitz matrices) where each row vector is rotated one element to the right relative to the preceding row vector.An $n \times n$ Circulant matrix C takes the form,

$$C = \begin{bmatrix} c_0 & c_{n-1} & \cdots & c_2 & c_1 \\ c_1 & c_0 & c_{n-1} & \ddots & c_2 \\ \vdots & c_1 & c_0 & \ddots & \vdots \\ c_{n-2} & \ddots & \ddots & \ddots & c_{n-1} \\ c_{n-1} & c_{n-2} & \cdots & c_1 & c_0 \end{bmatrix}$$

A Circulant matrix is fully specified by one vector, c, which appears as the first column of C. The remaining columns of C are each cyclic permutations of the vector c with offset equal to the column index. The last row of C is the vector c in reverse order, and the remaining rows are each cyclic permutations of the last row.

Note that difference source define circulant matrix in different way, for example with the coefficients corresponding to the first row rather than the first column of the matrix, or with a different direction of shift. The Eigen values of a Circulant matrix are given by $\lambda_j = c_0 + c_{n-1}\omega_j + c_{n-2}\omega_j^2 + ... + c_1\omega_j^{n-1}, \quad j = 0, ...n-1$ Where ω_j are the n th roots of unity and $i = \sqrt{-1}$ is the imaginary unit.

Lemma 3.2.1. If C is a Circulant matrix of order n with first row $a_1, a_2, ... a_n$ then the determinant of C is given by,

$detC = \prod_{0\leq j\leq n-1} a_1 + a_2\omega^j + a_3\omega^{2j} + ... + a_n\omega^{(n-1)j}$, where ω is the primitive n th root of unity.

3.3 Circulant graph

Let $S \subset 1, 2, . . . , n$ with the property that if $i \in S$ then $n - i \in S$. The graph G with the vertex set $V = \{v_0, v_1, ...v_{n-1}\}$ in which v_i adjacent to v_j if and only if $i - j(modn) \in S$, is called a circulant graph of order n.

Since the adjacency matrix $A(G)$ of G is a Circulant matrix of order n with 1 in the $(i + 1)$ th position of its first row if and only if $i \in S$ and zero in the remaining positions.

Clearly G is a $|S|$ regular graph, if $S = \{\alpha_1, \alpha_2, ...\alpha_n\}$ a subset of $\{1, 2, . . . , n\}$ then first row of $A(G)$ poses 1 in the $(\alpha_i + 1)$ th position for $1 \leq i \leq k$ and zero in the remaining positions. Hence by above lemma, the Eigen values are given by $\{\omega^{j\alpha_1} + \omega^{j\alpha_2} + ...\omega^{j\alpha_k} : 0 \leq j \leq n - 1, w = a$ primitive n th root of unity$\}$.

Definition 3.3.1. A Hamilton graph is a graph with a spanning cycle, it is also called a **Hamilton cycle**.

Example of non hyper energetic graph

Example 3.3.1. All graph of order n with number of edges less than $2n - 2$ are non hyper-energetic

Definition 3.3.2. A subdivision graph $S(G)$ of a graph G is obtained by inserting a new vertex on each edge of G. Hence if G has n vertices and m edges then its subdivision graph $S(G)$ has $m + n$ vertices and $2m$ edges.

Example 3.3.2. All subdivision graphs are non-hyperenergetic. Recall that the subdivision graph $S(G)$ of a graph G is obtained by inserting a new vertex on each edges of G.

Hence if G has n vertices and m edges,$S(G)$ has $m + n$ vertices and $2m$ edges. Now all graphs of order n with number of edges less than $2n - 2$ are non-hyper-energetic.For all subdivision graph of non-trivial graph, we have

$$2m < 2|V(S(G))| - 2 = 2(m + n) - 2$$

Hence all subdivision graphs are non-hyperenergetic

Chapter 4

Energy Bounds

For a graph G on n vertices and having m edges, it's shown in the research paper [6] that

$$E(G) \leq \frac{2m}{n} + \sqrt{n-1\left[2m - \left(\frac{2m}{n}\right)^2\right]} = B_1 \qquad (4.1)$$

Now consider a k-regular graph, then we have the number of edges of this k-regular graph is $m = \frac{nk}{2}$, apply this in the above equation, then we will get

$$\begin{aligned} E(G) &\leq \frac{2\frac{nk}{2}}{n} + \sqrt{(n-1)\left[2\frac{nk}{2} - \left(\frac{2(\frac{nk}{2})}{n}\right)^2\right]} \\ &= \frac{2nk}{2n} + \sqrt{(n-1)\left[\frac{2nk}{2} - \left(\frac{2nk}{2n}\right)^2\right]} \\ &= k + \sqrt{(n-1)(nk-k^2)} = B_2 \ (say) \qquad (4.2) \end{aligned}$$

This is for a k-regular graph G of order n, $E(G) \leq k + \sqrt{k(n-1)(n-k)} = B_2$

4.1 Cubic Graph

Definition 4.1.1. **Cubic graph** is a graph that is a regular of degree 3. from (4.2) and this definition, we shall obtain the following result.

Result 4. All cubic graphs are non hyper-energitic.

Proof. We know that a cubic graph is a 3-regular graph. Now consider the upper energy bound $B_2 = k + \sqrt{k(n-1)(n-k)}$ of a k-regular graph and put $k = 3$, $B_2 = 3 + \sqrt{3(n-1)(n-3)}$

Now,

$$B_2 \le 2(n-1) \tag{4.3}$$

$$\Rightarrow 3 + \sqrt{3(n-1)(n-3)} \le 2(n-1)$$

$$\Rightarrow \sqrt{3(n-1)(n-3)} \le 2n-5$$

$$\Rightarrow 3(n-1)(n-3) \le (2n-5)^2$$

$$\Rightarrow 3(n^2-4n+3) \le 4n^2-20n+25$$

$$\Rightarrow 0 \le n^2-8n+16$$

$$\Rightarrow 0 \le (n-4)^2 \tag{4.4}$$

Now since (4.4) is true, we get that (4.3) is also true that is $B_2 \le 2(n-1)$. So $E(G) \le B_2 \le 2(n-1)$ this implies that G is non hyper energitic. Therefore we can conclude that every cubic graph is non hyper-energitic. □

Note: There are regular for which the bound B_2 is attained.

To see this, consider the complete graph K_n, clearly K_n is a $(n-1)$ regular graph.so

$$\begin{aligned} B_2 &= k + \sqrt{k(n-1)(n-k)} \\ &= (n-1) + \sqrt{(n-1)(n-2)(n-(n-1))} \\ &= (n-1) + (n-1) \\ &= 2(n-1) \end{aligned}$$

Also we have $E(K_n) = 2(n-1)$. i.e, we got that $E(K_n) = B_2$. Showing that both B_1 and B_2 are sharp bound for the energy concept of a simple graph.

Lemma 4.1.1. For any two positive integer n and k, $n-1 > k \geq 2$ and $\epsilon > 0$, does there exist a k-regular graph G with $\frac{E(G)}{B_2} > 1-\epsilon$, where $B_2 = k + \sqrt{k(n-1)(n-k)}$

Proof. We know $E(G) \leq B_2$. For $\epsilon > 0$ we can write $E(G) + \epsilon = B_2$. By the condition $n-1 > k \geq 2$, it is clear B_2 always greater than 1. Then $E(G) + \epsilon > 1$

$$\begin{aligned} E(G) &> 1-\epsilon \\ \Longrightarrow \frac{E(G)}{B_2} &> 1 > \frac{1-\epsilon}{B_2} \end{aligned}$$

As $B_2 > 1$

$$\Longrightarrow \frac{E(G)}{B_2} > 1-\epsilon$$

□

Recently J. H. Koolen and V. Moulton in papers maximal energy graphs [8] and maximal energy bipartite graph [7] showed that for a graph G with n vertices and m edges

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)(2m - \frac{4m^2}{n^2})} \tag{4.5}$$

And for bipartite graph with n vertices and m edges

$$E(G) \leq \frac{4m}{n} + \sqrt{(n-2)(2m - \frac{4m^2}{n^2})}$$

And characterized those graphs for which these bounds are best possible. Then they proved that for graph G with n vertices

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

And for bipartite graph G with n vertices

$$E(G) \leq \frac{n}{\sqrt{8}}(\sqrt{n} + \sqrt{2})$$

And those graphs for which these bounds are best possible can be characterized.

4.2 Semi regular bipartite Graph

Definition 4.2.1. A graph G is **semi regular bipartite** (of degree r_1 and r_2) if it is bipartite and each in the same part of bipartition has the same degree (each vertex in one part of bipartition has degree r_1 and each vertex in the other part of bipartition has degree r_2)

Clearly a regular bipartite graph is a semi-regular bipartite graph with $r_1 = r_2$ If $\lambda_1 \geq \lambda_2 \geq .... \geq \lambda_n$ eigen values of G among the known lower bounds of λ_1 [5] is the following

$$\lambda_1 \geq \sqrt{\frac{\sum_i d_i^2}{n}} \tag{4.6}$$

And the equality holds if and only if G is a regular bipartite graph, where $d_1, d_2, ..., d_n$ the degree sequence of G. The degree sequence of a graph G is the list of vertex degrees, usually written in non increasing order, as $d_1 \geq d_2 \geq ... \geq d_n$

4.3 Strongly regular Graph

Definition 4.3.1. A **strongly regular graph**G with parameters (n, k, ρ, σ) is a k-regular graph on n vertices each pair of adjacent vertices has ρ common neighbors and each pair of non adjacent vertices has σ common neighbors.

If $\sigma = 0$, then G is a disjoint union of complete graph, whereas if $\sigma \geq 1$ and G is non-complete, then the Eigen values of G are k, s and t with multiplicities 1, m_s and m_t where s, t are the root $x^2 + (\sigma - \rho)x + (\sigma - k) = 0$, this because a theorem from graph theory. A k-regular connected graph G is strongly regular with parameters n, k, ρ, σ and only if it has exactly 3 Eigen values k, s and t such that $k > s > t$ and these satisfies $s + t = \rho - \sigma$ and $st = \rho - k$. i.e s, t are roots of $x^2 + (\sigma - \rho)x + (\sigma - k) = 0$ and m_s and m_t are determined by $m_s + m_t = n - 1$ (sum of the multiplicities of Eigen values of a graph G is the order of G) and $k + m_s s + m_t t = 0$ (sum of the Eigen values of a simple graph = trace A = 0).

Theorem 4.3.1. If G is a graph with n vertices, m edges and degree sequence $d_1, d_2, \ldots d_n$ then,

$$E(G) \leq \sqrt{\frac{\sum_i d_i^2}{n}} + \sqrt{(n-1)\left(2m - \frac{\sum_i d_i^2}{n}\right)} \tag{4.7}$$

Moreover the equality holds if and only if G either

1. $\frac{n}{2}K_2 \quad (m = \frac{n}{2})$
2. $K_n \quad (m = \frac{n(n-1)}{2})$
3. A non-complete connected strongly regular graph with two non trivial Eigen values both with absolute value $\sqrt{\frac{2m-(\frac{2m}{n})^2}{n-1}}$, or
4. nk_1 $(m = 0)$

Proof. Let G be a graph with Eigen values $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ recall (4.6). That is, among the known lower bounds of λ_1 is the following $\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^n d_i^2}{n}}$ where $d_1, d_2, \ldots d_n$ the degree sequence of G. Then by Cauchy-schwartz inequality we have

$$\sum_{i=2}^n |\lambda_i| \leq \sqrt{(n-1)\sum_{i=2}^n \lambda_i^2} = \sqrt{(n-1)\left(\sum_{i=1}^n \lambda_i^2 - \lambda_1^2\right)}$$

Then since $\sum \lambda_i^2 = 2m = traceA^2$, we have

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