

A note on energy of some graphs

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Abstract

Eigenvalue of a graph is the eigenvalue of its adjacency matrix. The energy $\mathcal{E}(G)$ of a graph G is the sum of the absolute values of its eigenvalues. In this paper we obtain analytic expressions for the energy of two classes of regular graphs.

1 Introduction

Let G be a graph with $|V(G)| = p$ and an adjacency matrix A . The eigenvalues of A are called the eigenvalues of G and form the spectrum of G denoted by $spec(G)$ [3]. The energy [6] of G , $\mathcal{E}(G)$ is the sum of the absolute values of its eigenvalues.

From the pioneering work of Coulson [2] there exists a continuous interest towards the general mathematical properties of the total π -electron energy \mathcal{E} as calculated within the framework of the Hückel Molecular Orbital (HMO) model [7]. These efforts enabled one to get an insight into the dependence of \mathcal{E} on molecular structure. The properties of $\mathcal{E}(G)$ are discussed in detail in [6, 8, 9].

In [5] the spectra and energy of several classes of graphs containing a linear polyene fragment are obtained. In [12], we obtain the energy of cross products of some graphs. In [15], the energy of iterated line graphs of regular graphs and in [13], the energy of some self-complementary graphs are discussed. The energy of regular graphs are discussed in [10]. Some other works pertaining to the computation of $\mathcal{E}(G)$ can be seen in [1, 4, 6, 11, 14].

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As there is no easy way to find the eigenvalues of a graph G , the computation of the actual value of $\mathcal{E}(G)$ is an interesting problem in graph theory. In this note we obtain analytic expressions for the energy of two classes of regular graphs.

All graph theoretic terminology is from [3]. We use the following lemmas and definitions in this paper.

Lemma 1. [3] *Let M, N, P and Q be matrices with M invertible. Let*

$$S = \begin{bmatrix} M & N \\ P & Q \end{bmatrix}. \text{ Then, } |S| = |M| |Q - PM^{-1}N| \text{ and if } M \text{ and } P \text{ commutes, then, } |S| = |MQ - PN|$$

where the symbol $|\cdot|$ denotes the determinant.

Lemma 2. [3] *Let G be an r -regular connected graph on p vertices with A as an adjacency matrix and $r = \lambda_1, \lambda_2, \dots, \lambda_m$ as the distinct eigenvalues. Then there exists a polynomial $P(x)$ such that $P(A) = J$ where J is the all one square matrix of order p and $P(x)$ is given by $P(x) = p \times \frac{(x-\lambda_2)(x-\lambda_3)\dots(x-\lambda_m)}{(r-\lambda_2)(r-\lambda_3)\dots(r-\lambda_m)}$, so that $P(r) = p$ and $P(\lambda_i) = 0$, for all $\lambda_i \neq r$.*

Lemma 3. [3] $\text{spec}(C_p) = \begin{pmatrix} 2 & 2 \cos \frac{2\pi}{p} j \\ 1 & 1 \end{pmatrix}$ and $\text{spec}(\overline{C_p}) = \begin{pmatrix} p-3 & -1 - 2 \cos \frac{2\pi}{p} j \\ 1 & 1 \end{pmatrix}$,

$j = 1$ to $p-1$.

Lemma 4. [3] *Let G be an r -regular graph with an adjacency matrix A and incidence matrix R . Then, $RR^T = A + rI$.*

Definition 1. *Let G be a (p, q) graph. The complement of the incidence matrix R , denoted by $\overline{R} = [\overline{r}_{ij}]$ is defined by*

$$\begin{aligned} \overline{r}_{ij} &= 1 \text{ if } v_i \text{ is not incident with } e_j \\ &= 0, \text{ otherwise.} \end{aligned}$$

Definition 2. *Let G be a (p, q) graph. Corresponding to every edge e of G introduce a vertex and make it adjacent with all the vertices not incident with e in G . Delete the edges of G only. The resulting graph is called the partial complement of the subdivision graph of G , denoted by $\overline{S}(G)$.*

2 Partial complement of the subdivision graph

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

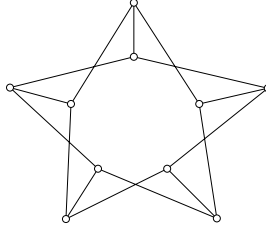


Figure 1: $\overline{S}(C_5)$

Lemma 5. Let G be an r -regular (p, q) graph with an adjacency matrix A and incidence matrix R . Then, $\overline{R} = J_{p \times q} - R$, $\overline{R}^T = J_{q \times p} - R^T$ and $\overline{R}\overline{R}^T = (q - 2r)J + (A + r)$ where J is the all one matrix of appropriate order.

Proof. By Definition 1, $\overline{R} = J_{p \times q} - R$. Therefore

$$\begin{aligned} \overline{R}\overline{R}^T &= (J_{p \times q} - R)(J_{q \times p} - R^T) \\ &= qJ - rJ - rJ + A + rI \\ &= (q - 2r)J + (A + r)I, \text{ by Lemma 4.} \end{aligned}$$

Hence the lemma. □

Lemma 6. Let G be a connected r -regular (p, q) graph. Then, $\overline{S}(G)$ is regular if and only if G is a cycle.

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

Theorem 1. Let G be a connected r -regular (p, q) graph. Then,

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

Proof. The adjacency matrix of $\overline{S}(G)$ can be written as $\begin{bmatrix} 0 & \overline{R} \\ \overline{R}^T & 0 \end{bmatrix}$. Then, the theorem follows from Lemmas 1 and 5. □

Theorem 2.

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

Proof. By Lemma 3 and Theorem 1 we have

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

We shall consider the following two cases.

Case 1. $p \equiv 0 \pmod{2}$.

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

$$\begin{aligned} \text{Let } C &= 2 \cos \frac{\pi}{p} + 2 \cos \left(\frac{\pi}{p} \times 2\right) + \dots + 2 \cos \left(\frac{\pi}{p} \times \frac{p}{2}\right) \text{ and} \\ S &= 2 \sin \frac{\pi}{p} + 2 \sin \left(\frac{\pi}{p} \times 2\right) + \dots + 2 \sin \left(\frac{\pi}{p} \times \frac{p}{2}\right) \end{aligned}$$

so that

$$\begin{aligned} C + iS &= 2\gamma + 2\gamma^2 + \dots + 2\gamma^{\frac{p}{2}} \\ &= 2\gamma \frac{(1 - \gamma^{\frac{p}{2}})}{1 - \gamma} \text{ where } \gamma = \cos \frac{\pi}{p} + i \sin \frac{\pi}{p} \text{ and } i = \sqrt{-1}. \end{aligned}$$

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

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

Case 2. $p \equiv 1 \pmod{2}$.

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

3 Energy of the complement of a cycle.

In [5], I.Gutman obtained an analytic expression for the energy of a cycle C_p . In this section we derive the energy of $\overline{C_p}$, the complement of the cycle C_p .

Theorem 3.

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

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

We shall consider the following cases.

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

Then, $-\left(1+2 \cos \frac{2\pi j}{p}\right) \geq 0$ if and only if $\frac{p}{3} \leq j \leq \frac{2p}{3}$.

Let $\sum_{j=\frac{p}{3}}^{\frac{2p}{3}} \left(1+2 \cos \frac{2\pi j}{p}\right) = \frac{p+3}{3} + \sum_{j=\frac{p}{3}}^{\frac{2p}{3}} 2 \cos \frac{2\pi j}{p} = \frac{p+3}{3} + C$ and

$S = \sum_{j=\frac{p}{3}}^{\frac{2p}{3}} 2 \sin \frac{2\pi j}{p}$, so that $C + iS = \sum_{j=\frac{p}{3}}^{\frac{2p}{3}} \gamma^j$ where $\gamma = \cos \frac{2\pi}{p} + i \sin \frac{2\pi}{p}$.

Equating real parts, we get $C = -(1 + \sqrt{3} \cot \frac{\pi}{p})$.

The total sum of positive eigenvalues

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

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

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

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