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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* $S = \begin{bmatrix} M & N \\ P & Q \end{bmatrix}$. *Then, $|S| = |M|\left|Q - PM^{-1}N\right|$ and if M and P commutes, then, $|S| = |MQ - PN|$ where the symbol $|.|$ denotes the determinant.*

Lemma 2. *[3] Let G be an $r-$ regular connected graph on p vertices with A as an adjacency matrix and $r = \lambda_1, \lambda_2, \ldots, \lambda_m$ 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 $P(x) = p \times \frac{(x-\lambda_2)(x-\lambda_3)\ldots(x-\lambda_m)}{(r-\lambda_2)(r-\lambda_3)\ldots(r-\lambda_m)}$, so that $P(r) = p$ and $P(\lambda_i) = 0$, for all $\lambda_i \neq r$.*

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

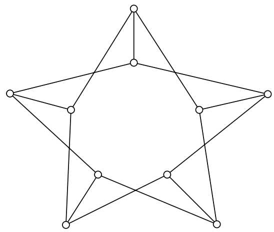

Figure 1: $\overline{S}(C_5)$

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 $R\overline{R}^T = (q-2r)\,J + (A+r)$ where J is the all one matrix of appropriate order.*

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

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

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,*

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

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.

$$\mathcal{E}\left(\overline{S}\left(C_p\right)\right) = \begin{cases} 2\left(p-4+2\cot\frac{\pi}{2p}\right), p \equiv 0(mod2) \\ \\ 2\left(p-4+2cosec\ \frac{\pi}{2p}\right), p \equiv 1(mod2) \end{cases}$$

Proof. By Lemma 3 and Theorem 1 we have

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

We shall consider the following two cases.

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

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

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

so that

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

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

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

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

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

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

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

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

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

The total sum of positive eigenvalues

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

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

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

References

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

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

[3] D.M.Cvetkovic, M. Doob, H. Sachs, *Spectra of Graphs-Theory and Applications*, Academic Press, (1980).

[4] I. Gutman, M. Milun, N. Trinajstić, *Hückel Molecular Orbital Calculations of Aromatic Stabilization of Annulenes*, Croat. Chem. Acta, **44** (1972), 207-213.

[5] I. Gutman, *A graph theoretical study of conjugated systems containing a linear polyene fragment*, Croat. Chem. Acta, **48(2)**(1976), 97 - 108.

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

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

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

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

[10] I. Gutman, S. Zare Firoozabadi, J. A. de la Peña, J. Rada, *On the energy of regular graphs*, MATCH Commun. Math. Comput. Chem., **57** (2007), 435-442.

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

[12] G. Indulal, A. Vijayakumar, *Energies of some non-regular graphs*, J. Math. Chem., (to appear).

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

[14] O. E. Polansky, *Über ungesättigte monocyclen mit durchlaufender konjugation, 2. Mitt.: Berechnung der elektronenstruktur mit hilfe der einfachen LCAO-MO-Methode und allgemeine gruppentheoretische betrchtungen*, Monatsh. Chem., **91** (1960), 916-962

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