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SOME RECURRENCE RELATIONS FOR THE ENERGY OF CYCLE AND PATH GRAPHS

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ABSTRACT. Energy of a graph, first defined by E. Hückel as the sum of absolute values of the eigenvalues of the adjacency matrix while searching for a method to obtain approximate solutions of Schrödinger equation for a class of organic molecules, is an important sub area of graph theory. This equation is a second order differential equation which include the energy of the corresponding system. The energy of many graph types are well-known in literature. To know the energy of a molecule is an important aspect in Chemical Graph Theory. Two classes, cycles and paths, show serious differences from others as the eigenvalues are trigonometric algebraic numbers which makes it difficult to calculate the energy of the corresponding graph. Here we obtain the polynomials and recurrence relations for the spectral polynomials of cycles and paths to find the energy of larger graphs easier than the classical way.

1. INTRODUCTION

Throughout this paper, we will take $G = (V, E)$ as a simple connected and undirected graph. The word simple means that G is a graph with no loops nor multiple edges. We call two vertices u and v of G adjacent if there is an edge e of G connecting u to v. If G has n vertices $v_1, v_2, \cdots, v_n$, we can form an $n \times n$ matrix $A = (a_{ij})$ by

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

This very useful matrix is called the adjacency matrix of the graph G. As well-known, the eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_n$ of a square $n \times n$ matrix A, which we shall also call as the eigenvalues of the graph G, are the roots of the equation $|A - \lambda I_n| = 0$. The polynomial on the left hand side of this equation is

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called the characteristic (or spectral) polynomial of A (and of the graph G). The set of all eigenvalues of the adjacency matrix A is called the spectrum of the graph G, denoted by $S(G)$. For more detailed information about the fundamental topics on graphs and spectrums of some well-known graphs, see [2], [8], [4], [5], [6], [12], [14], [15], [17], [18] and [23].

The sum of absolute values of the eigenvalues of G which was defined for the first time by E. Hückel in [19] is called the energy of G, which is an important aspect for the subfield of graph theory called spectral graph theory, and also for the molecular calculations, see [1], [13], [8], [16], [20], [21], [22].

As usual, we denote a path graph by P_n and a cycle graph by C_n. The spectrum of these graphs are known in literature, [20], [8]. These two spectra show differences with the other graph types as these two are the only ones which can be stated in terms of the roots of unity. The authors, in [10], found the characteristic polynomials of some graph types including path and cycle graphs, and also gave the recurrence formulae for these graph polynomails. In [11], the authors studied the spectrum of path and cycle graphs and find these spectra in terms of spectra of smaller graphs of the same type. In particular, they gave the spectrum of P_{2n+1} in terms of the spectrum of P_n, and the spectrum of C_{2n} in terms of the spectrum of C_n. These allow us to find more complicated spectra by means of easier spectra.

In this paper, we give some further relations for the spectrum and the energy of the cyclic, path, complete bipartite, complete and star graphs. Especially we obtain a very short formula for the energy of C_{2^m}.

2. Energy of Cycle Graphs and Their Recurrences

It is known that the spectrum of a cycle graph C_n is given by

$$S(C_n) = \left\{ \lambda_i : \lambda_i = 2\cos\left(\frac{2\pi i}{n}\right), \quad i = 0, 1, 2, \ldots, n-1 \right\}$$

see [8], [20], [10]. If we note that the elements of $S(C_n)$ are all algebraic numbers defined by means of trigonometrical functions, then we can obtain the eigenvalues of some cycle graph in terms of the eigenvalues of a smaller cycle graph. We first recall the following useful result from [11]:

Lemma 2.1. *Let C_n be a cycle graph. Then for every $k = 1, 2, \ldots, n-1$,*

$$\lambda_k = \lambda_{n-k}.$$

Lemma 2.1 enables one to calculate only $\lambda_0, \lambda_1, \ldots, \lambda_{[|n/2|]}$ instead of calculating all $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$ as follows:

For $n \geq 3$, let the spectrum of C_n be

$$S(C_n) = \{\lambda_0, \lambda_1, \ldots, \lambda_{n-2}, \lambda_{n-1}\}$$

and the spectrum of C_{2n} be

$$S(C_{2n}) = \{\mu_0, \mu_1, \ldots, \mu_{2n-2}, \mu_{2n-1}\}.$$

For $j = 0, 1, \cdots, 2n-1$, the relation between λ_i's and μ_j's is given in [11]:

$$\mu_{2j} = 2\cos\left(\frac{2\pi 2j}{2n}\right) = 2\cos\left(\frac{2\pi j}{n}\right) = \lambda_j.$$

Also, using double angle formulae, we have for every $k = 1, 2, \ldots, n-1$ that

$$\mu_k = \mu_{2n-k} = \mp\sqrt{\lambda_k + 2}.$$

Theorem 2.1. *For $m \geq 3$,*

$$\begin{aligned} E(C_{2^m}) &= 4\left(1 + \sqrt{2} + 2\sqrt{\sqrt{2}+2} + 4\sqrt{\sqrt{\sqrt{2}+2}+2} \right. \\ &\qquad \left. + \cdots + 2^{m-3}\sqrt{\sqrt{\ldots\sqrt{\sqrt{2}+2}+2+\ldots}+2}\right) \end{aligned}$$

where there are $m-2$ square roots in the last term.

Proof. By induction. For $m = 3$, let the spectrum of C_8 be $\{\mu_0, \mu_1, \mu_2, \cdots, \mu_7\}$. Recall that C_4 has the spectrum $\{\lambda_0 = 2, \lambda_1 = 0, \lambda_2 = -2, \lambda_3 = 0\}$. By the proof of Theorem 2.1 in [11],

$$\mu_0 = \lambda_0 = 2,\ \mu_2 = \lambda_1 = 0,\ \mu_4 = \lambda_2 = -2,\ \mu_6 = \lambda_3 = 0$$

and

$$\mu_1 = \sqrt{\lambda_1 + 2},\ \mu_3 = \sqrt{\lambda_3 + 2},\ \ldots,\ \mu_7 = \sqrt{\lambda_7 + 2}.$$

Also $\mu_7 = \mu_1$ and $\mu_5 = \mu_3$ by [11]. Then

$$\begin{aligned} E(C_{2^3}) = \sum_{i=0}^{7} |\mu_i| &= |\mu_0| + |\mu_1| + |\mu_2| + |\mu_3| + |\mu_4| + |\mu_5| + |\mu_6| + |\mu_7| \\ &= |\lambda_0| + |\lambda_1| + |\lambda_2| + |\lambda_3| + 2(|\mu_1| + |\mu_3|) \\ &= E(C_4) + 2(\sqrt{\lambda_1 + 2} + \sqrt{\lambda_3 + 2}) \\ &= 4(1 + \sqrt{2}). \end{aligned}$$

Let the spectrum of C_{2^m} be $\{\alpha_0, \alpha_1, \alpha_2, \ldots, \alpha_{2^m-1}\}$ and the spectrum of $C_{2^{m-1}}$ be $\{\beta_0, \beta_1, \beta_2, \ldots, \beta_{2^{m-1}-1}\}$. Note that

$$\beta_{2k+1} = \sqrt{\sqrt{\ldots\sqrt{\sqrt{2}+2}+2+\ldots}+2},$$

where there are $m-3$ times successive square roots. Let

$$\begin{aligned} E(C_{2^{m-1}}) &= 4\Bigg(1 + \sqrt{2} + 2\sqrt{\sqrt{2}+2} + 4\sqrt{\sqrt{\sqrt{2}+2}+2} \\ &\qquad + \cdots + 2^{m-4}\sqrt{\sqrt{\sqrt{\ldots\sqrt{2}+2}+\ldots}+2}\Bigg). \end{aligned}$$

Then

$$\begin{aligned} E(C_{2^m}) &= \sum_{k=0}^{2^m-1} |\alpha_k| \\ &= \sum_{k=0}^{2^{m-1}-1} |\alpha_{2k}| + \sum_{k=0}^{2^{m-1}-1} |\alpha_{2k+1}| \\ &= \sum_{k=0}^{2^{m-1}-1} |\beta_k| + \sum_{k=0}^{2^{m-1}-1} \sqrt{\beta_{2k+1}+2} \\ &= 4\Bigg(1 + \sqrt{2} + 2\sqrt{\sqrt{2}+2} + 4\sqrt{\sqrt{\sqrt{2}+2}+2} \\ &\qquad + \cdots + 2^{m-3}\sqrt{\sqrt{\sqrt{\ldots\sqrt{2}+2}+\ldots}+2}\Bigg). \end{aligned}$$

This completes the induction step. □

There is an immediate result giving a recurrence formula for the energy of the cycle graphs:

Corollary 2.1. *The recurrence formula for the energy of the cycle graphs is given by*

$$E(C_{2^m}) = E(C_{2^{m-1}}) + 2^{m-1}\sqrt{\sqrt{\sqrt{\ldots\sqrt{2}+2}+\ldots}+2}.$$

Example 1. We want to calculate the energy of the cycle graph C_{64}. First by Theorem 2.1, we have

$$\begin{aligned} E(C_{64}) = E(C_{2^6}) &= 4\Bigg(1+\sqrt{2}+2\sqrt{\sqrt{2}+2}+2^2\sqrt{\sqrt{\sqrt{2}+2}+2} \\ &\quad + 2^3\sqrt{\sqrt{\sqrt{\sqrt{2}+2}+2}+2}\Bigg) \\ &\approx 119,496. \end{aligned}$$

It is easier to calculate the energy of the cycle graph C_{32} by Theorem 2.1:

$$E(C_{32}) \approx 55,808.$$

Then by Corollary 2.1, we can calculate $E(C_{64})$ by the recurrence formula:

$$\begin{aligned} E(C_{64}) = E(C_{2^6}) &= E(C_{2^5}) + 2^5\sqrt{\sqrt{\sqrt{\sqrt{2}+2}+2}+2} \\ &\approx 55,808 + 32\cdot 1,990 \\ &\approx 119,496. \end{aligned}$$

3. Recurrence Relations for the Energy of Some Graph Types

The energy of some special graph types are well-known in literature, see [9, 10, 20, 8]. In this section, we give recurrence relations for the path, cycle, star, complete and complete bipartite graphs by means of the known results on these references.

It is known that the energy of a complete graph K_n is given by

$$E(K_n) = 2(n-1).$$

The recurrence relation for the complete graph is given by,

Lemma 3.1. *Let $E(K_n)$ be the energy of the complete graph K_n. Then*

$$E(K_{2n-1}) = 2E(K_n).$$

Proof. By [9, 10, 20, 8], we have

$$\begin{aligned} E(K_{2n-1}) &= 2(2n-1-1) \\ &= 2(2n-2) \\ &= 2 \cdot 2(n-1) \\ &= 2E(K_n). \end{aligned}$$

□

Similarly, it is known that the energy of the star graph S_n is given by

$$E(S_n) = 2\sqrt{n-1}.$$

The recurrence relation for the star graph is given by the following:

Lemma 3.2. *Let $E(S_n)$ be the energy of the star graph. Then*

$$E(S_{2n-1}) = \sqrt{2}E(S_n).$$

Proof. Similarly to complete graphs, we have

$$\begin{aligned} E(S_{2n-1}) &= 2\sqrt{2n-1-1} \\ &= 2\sqrt{2n-2} \\ &= \sqrt{2} \cdot 2\sqrt{n-1} \\ &= \sqrt{2}E(S_n). \end{aligned}$$

□

The energy of the complete bipartite graph $K_{m,n}$ is given by

$$E(K_{m,n}) = 2\sqrt{m.n}.$$

The recurrence relation for this graph is given by the following result:

Lemma 3.3. *Let $E(K_{m,n})$ be the energy of the complete bipartite graph $K_{m,n}$. Then the recurrence relation is given by*

$$\begin{aligned} E(K_{2m,n}) &= E(K_{m,2n}) \\ &= \sqrt{2}E(K_{m,n}). \end{aligned}$$

Proof.

$$\begin{aligned} E(K_{2m,n}) &= E(K_{m,2n}) \\ &= 2\sqrt{2mn} \\ &= 2\sqrt{2}\sqrt{mn} \\ &= \sqrt{2}E(K_{m,n}). \end{aligned}$$

□

Corollary 3.1. *The reccurence relation for the energy of $K_{rm,sn}$ can be defined by*

$$E(K_{rm,sn}) = \sqrt{rs}E(K_{m,n}).$$

Proof.

$$\begin{aligned} E(K_{rm,sn}) &= 2\sqrt{rm \cdot sn} \\ &= 2\sqrt{rs}\sqrt{mn} \\ &= \sqrt{rs}E(K_{m,n}). \end{aligned}$$

□

See [8], [20], [10], the elements of $S(P_n)$ and $S(C_n)$, are all algebraic numbers defined by means of trigonometrical functions. For this reason, obtaining the reccurence relations for the energy of these graph types are more complicated than the others.

Theorem 3.1. *For $n \geq 3$, $S(C_n) = \{\lambda_0, \lambda_1, \ldots, \lambda_{n-1}\}$ then,*

$$\frac{E(C_{2n}) - E(C_n)}{2} = \begin{cases} \displaystyle\sum_{j=1}^{\frac{n}{2}} \sqrt{\lambda_{2j-1} + 2}, & for\ n\ is\ even \\ \displaystyle\sum_{j=1}^{\frac{n-1}{2}} \sqrt{\lambda_{2j-1} + 2}, & for\ n\ is\ odd. \end{cases}$$

Proof. It is well known that,

$$E(C_n) = \sum_{j=1}^{n-1} |\lambda_j|.$$

Also, the relation between the spectrum of $E(C_n)$ and $E(C_{2n})$ is given in [11]. Therefore, $E(C_{2n}) = E(C_n) + 2\sum_{j=1}^{[|n/2|]} \sqrt{\lambda_{2j-1}+2}$. Hence the result follows.

$$\frac{E(C_{2n}) - E(C_n)}{2} = \begin{cases} \sum_{j=1}^{\frac{n}{2}} \sqrt{\lambda_{2j-1}+2}, & for\ n\ is\ even \\ \sum_{j=1}^{\frac{n-1}{2}} \sqrt{\lambda_{2j-1}+2}, & for\ n\ is\ odd. \end{cases}$$

□

Similarly to The Theorem 3.1, we give the following result:

Theorem 3.2. *Let* $S(P_n) = \{\lambda_0, \lambda_1, \ldots, \lambda_{n-1}\}$ *then,*

$$\frac{E(P_{2n}) - E(P_n)}{2} = \begin{cases} \sum_{j=1}^{\frac{n}{2}} \sqrt{\lambda_{2j-1}+2}, & for\ n\ is\ even \\ \sum_{j=1}^{\frac{n-1}{2}} \sqrt{\lambda_{2j-1}+2}, & for\ n\ is\ odd. \end{cases}$$

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