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FORMULAE AND RECURRENCE RELATIONS ON SPECTRAL POLYNOMIALS OF SOME GRAPHS

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ABSTRACT. Energy of a graph, firstly 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. Schrödinger equation is a second order differantial equation which include the energy of the corresponding system. Here we obtain the polynomials and recurrence relations for the spectral (characteristic) polynomials of some graphs.

1. INTRODUCTION

Let $G = (V, E)$ be a simple connected graph, that is G is a graph with no loops nor multiple edges. Two vertices u and v of G are called 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 matrix is called the adjacency matrix of the graph G. The set of all eigenvalues of the adjacency matrix A is called the spectrum of the graph G, denoted by $S(G)$. These eigenvalues are also called the eigenvalues of the graph G. For more detailed information about the fundamental topics on graphs, see [2], [5], [6], [7], [10], [11], [12], [14], [15] and [19].

As well-known, the eigenvalues of a square $n \times n$ matrix A are the roots of the equation $|A - \lambda I_n| = 0$. The polynomial on the left hand side of this equation is called the characteristic polynomial of A (and of the graph G). For our aim, we shall call this polynomial the spectral polynomial of G. The sum of absolute values of the eigenvalues of G is called the energy of G, which is an important aspect for the subfield of graph theory called spectral graph theory, see [1], [3],

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[9], [13], [16], [17], [18].

As usual, we denote path, cycle, star, complete and complete bipartite graphs by P_n, C_n, S_n, K_n and $K_{r,s}$, respectively.

Figure 1.1 Path graph P_n

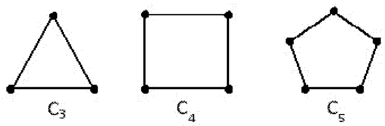

Figure 1.2 Cycle graphs C_3, C_4, C_5

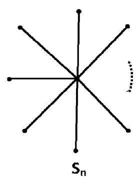

Figure 1.3 Star graph S_n

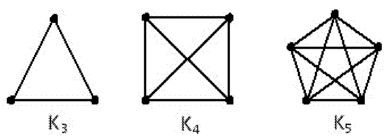

Figure 1.4 Complete graphs K_3, K_4, K_5

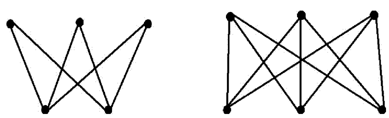

Figure 1.5 Complete bipartite graphs $K_{2,3}$ and $K_{3,3}$

2. Spectrum of Some Graph Types

The spectrum of some graph types including path, cycle, star, complete and complete bipartite graphs are known in literature. The spectrum of path and cycle graphs show differences with the other graph types as they can be stated in terms of roots of unity. In this section, we will reobtain the spectrum of these graph types by means of the characteristic polynomial. We shall give exact formulae for the spectral polynomials and also the recurrence relations for these polynomials, [4].

Let G be a graph. Let A denote the adjacency matrix of G. The solutions $\lambda_1, \lambda_2, ..., \lambda_n$ of the equation

$$|A - \lambda I_n| = 0$$

are the eigenvalues of the matrix A. We shall also call them the eigenvalues of the graph G. The set of all eigenvalues of G is called the spectrum of G. The sum of the absolute values of all eigenvalues of G is called the energy of G, denoted by $E(G)$. The notion of energy plays an important role in molecular calculations.

Here we shall focus on the polynomial $|A - \lambda I_n|$ and we call it the spectral polynomial of G. It will be denoted by $Pol(G)$.

The spectrum of some special graph types are well-known in literature, see [9].

Firstly we shall obtain the spectral polynomial $Pol(P_n)$ of a path graph P_n.

Theorem 2.1. *The spectral polynomial of P_n satisfies the following recurrence formula:*

$$Pol(P_n) = -\lambda Pol(P_{n-1}) \; - \; Pol(P_{n-2})$$

Proof. The adjacency matrix of P_n is

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & \dots & 0 \\ 1 & 0 & 1 & 0 & \dots & 0 \\ 0 & 1 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 \end{bmatrix}_{nxn} .$$

Therefore the spectral polynomial of P_n is given by

$$Pol(P_n) = |A - \lambda I_n|$$

$$= \begin{vmatrix} -\lambda & 1 & 0 & \dots & 0 \\ 1 & -\lambda & 1 & \dots & 0 \\ 0 & 1 & -\lambda & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -\lambda \end{vmatrix}_{n\times n}.$$

If we expand this determinant by the first row, we obtain

$$= -\lambda \begin{vmatrix} -\lambda & 1 & 0 & \dots & 0 \\ 1 & -\lambda & 1 & \dots & 0 \\ 0 & 1 & -\lambda & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -\lambda \end{vmatrix}_{(n-1)\times(n-1)} - \begin{vmatrix} 1 & 1 & 0 & \dots & 0 \\ 0 & -\lambda & 1 & \dots & 0 \\ 0 & 1 & -\lambda & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -\lambda \end{vmatrix}_{(n-1)\times(n-1)}.$$

Here, the first determinant is equal to $Pol(P_{n-1})$. If we expand the second determinant by the first column, we obtain

$$Pol(P_n) = -\lambda Pol(P_{n-1}) - \begin{vmatrix} -\lambda & 1 & 0 & \dots & 0 \\ 1 & -\lambda & 1 & \dots & 0 \\ 0 & 1 & -\lambda & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -\lambda \end{vmatrix}_{(n-2)\times(n-2)}.$$

This last determinant is equal to $Pol(P_{n-2})$. The result then follows. □

Using this result, we can obtain an exact formula for the spectral polynomial of P_n:

Theorem 2.2. *The spectral polynomial of P_n can be given by the following formula:*

- *if n is even,*

$$Pol(P_n) = \sum_{k=0}^{\frac{n}{2}} (-1)^k \binom{n-k}{k} \lambda^{n-2k}$$

- *if n is odd,*

$$Pol(P_n) = \sum_{k=0}^{\frac{n-1}{2}} (-1)^{k+1} \binom{n-k}{k} \lambda^{n-2k}$$

Proof. The proof can be seen by mathematical induction and the previous theorem. □

It is well-known that the roots of $Pol(P_n)$ are

$$\lambda_i = \cos\left(\frac{\pi i}{n+1}\right), \quad i = 1, 2, 3, \ldots, n,$$

see, [9]. Therefore the spectrum of $Pol(P_n)$ is

$$S(P_n) = \left\{\lambda_i : \lambda_i = \cos\left(\frac{\pi i}{n+1}\right), \quad i = 1, 2, 3, \ldots, n\right\}.$$

Secondly we calculate the spectral polynomial and exact formula for $Pol(K_n)$.

Theorem 2.3. *The spectral polynomial of K_n satisfies the following recurrence formula:*

$$Pol(K_n) = -\lambda Pol(K_{n-1}) \; - \; (n-1)\,(-\lambda - 1)^{n-2}$$

Proof. The adjacency matrix of K_n is

$$A = \begin{bmatrix} 0 & 1 & 1 & \ldots & 1 \\ 1 & 0 & 1 & \ldots & 1 \\ 1 & 1 & 0 & \ldots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \ldots & 0 \end{bmatrix}_{n\times n}.$$

Therefore the spectral polynomial of K_n is given by

$$Pol(K_n) = |A - \lambda I_n|$$

$$= \begin{vmatrix} -\lambda & 1 & 1 & \ldots & 1 \\ 1 & -\lambda & 1 & \ldots & 1 \\ 1 & 1 & -\lambda & \ldots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \ldots & -\lambda \end{vmatrix}_{n\times n}.$$

If we expand this determinant by the first column, we obtain

$$= -\lambda \begin{vmatrix} -\lambda & 1 & 1 & \dots & 1 \\ 1 & -\lambda & 1 & \dots & 1 \\ 0 & 1 & -\lambda & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & -\lambda \end{vmatrix}_{(n-1)\times(n-1)} - \begin{vmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & -\lambda & 1 & \dots & 1 \\ 1 & 1 & -\lambda & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & -\lambda \end{vmatrix}_{(n-1)\times(n-1)} .$$

$$= -\lambda Pol(K_{n-1}) - (n-1) \begin{vmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & -\lambda & 1 & \dots & 1 \\ 1 & 1 & -\lambda & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & -\lambda \end{vmatrix}_{(n-1)\times(n-1)} . \tag{2.1}$$

When the first row of this last determinant multiplied by -1 and added to other rows, the determinant becomes

$$\begin{vmatrix} (-1-\lambda) & 0 & 0 & \dots & 0 \\ 0 & (-1-\lambda) & 0 & \dots & 0 \\ 0 & 0 & (-1-\lambda) & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & (-1-\lambda) \end{vmatrix}_{(n-2)\times(n-2)}$$

which has the value $(-1-\lambda)^{n-2}$. If we substitute this value in equation (2.1), we get the following recurrence relation:

$$Pol(K_n) = -\lambda Pol(K_{n-1}) \ - \ (n-1)\,(-\lambda-1)^{n-2}$$

□

It is easy to show similarly that $Pol(K_n)$ can also be obtained by the following three-term recurence relation:

Corollary 2.3.1. $Pol(K_n) = -(\lambda+n-1)Pol(K_{n-1}) - (n-1)(\lambda+1)Pol(K_{n-2})$.

By repeated use of Theorem 2.3, we obtain a direct formula for $Pol(K_n)$:

Theorem 2.4. *The polynomial of K_n can be given by the following formula:*

$$Pol(K_n) = (-1)^k(\lambda+1)^{n-1}(\lambda-n-1).$$

According to Theorem 2.4, the spectrum of K_n is

$$S(K_n) = \{n-1, -1^{(n-1)}\}.$$

Thirdly, using similar calculations we obtain following results:

Theorem 2.5. *The spectral polinomial of S_n satisfies the following recurrence formula:*

$$Pol(S_n) = -\lambda Pol(S_{n-1}) - (-\lambda)^{n-2}.$$

Theorem 2.6. *The spectral polynomial of S_n can be given by the following formula:*

$$Pol(S_n) = (-\lambda)^{n-2}(\lambda^2 - n + 1).$$

By Theorem 2.6, it is obvious that the spectrum of S_n is

$$S(S_n) = \{\mp\sqrt{n-1},\ 0^{(n-2)}\}.$$

Proceeding similary for $K_{m,n}$ and C_n, we obtain the following results:

Theorem 2.7. *The spectral polynomial of $K_{m,n}$ satisfies the following recurrence formula:*

$$Pol(K_{m,n}) = -\lambda Pol(K_{m-1,n}) + (-1)^{m+n-1}\lambda^{m+n-2}n, \quad m > 1$$

and

$$Pol(K_{1,n}) = -\lambda Pol(K_{1,n-1}) - (-\lambda)^{n-1}, \quad m = 1.$$

Theorem 2.8. *The spectral polynomial of $K_{m,n}$ can be given by the following formula:*

$$Pol(K_{m,n}) = (-1)^{m+n}\lambda^{m+n-2}(\lambda^2 - mn).$$

By Theorem 2.8, the spectrum of $K_{m,n}$ is

$$S(K_{m,n}) = \{\mp\sqrt{mn},\ 0^{(m+n-2)}\}.$$

Finally, proceeding similarly, we obtain the spectral polynomial of C_n as follows:

Theorem 2.9. *The spectral polynomial of C_n satisfies the following recurrence formula:*

$$Pol(C_n) = -\lambda Pol(C_{n-1}) - Pol(C_{n-2}) + (-1)^n Pol(C_1)$$

It then follows that the spectrum of $Pol(C_n)$ is

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

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