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The normalized Laplacians, degree-Kirchhoff index and the spanning trees of linear hexagonal chains[☆]

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ABSTRACT

Let L_n be a linear hexagonal chain with n hexagons. In this paper, according to the decomposition theorem of normalized Laplacian polynomial of a graph, we obtain that the normalized Laplacian spectrum of L_n consists of the eigenvalues of two symmetric tridiagonal matrices of order $2n+1$. Together with the relationship between the roots and coefficients of the characteristic polynomials of the above two matrices, explicit closed formula of the degree-Kirchhoff index (resp. the number of spanning trees) of L_n is derived. Finally, it is interesting to find that the degree-Kirchhoff index of L_n is approximately one half of its Gutman index.

1. Introduction

In this paper, we consider simple and finite graphs only and assume that all graphs are connected, and refer to Bondy and Murty [3] for notation and terminologies used but not defined here.

Let $G = (V_G, E_G)$ be a graph with vertex set V_G and edge set E_G. The *adjacency matrix* $A(G)$ of G is a $|V_G| \times |V_G|$ matrix whose (i, j)-entry is equal to 1 if vertices v_i and v_j are adjacent and 0 otherwise. Let $D(G) = \mathrm{diag}(d_1, d_2, \ldots, d_{|V_G|})$ be the diagonal matrix, where d_i is the degree of v_i in G for $1 \leqslant i \leqslant |V_G|$. The (*combinatorial*) *Laplacian matrix* of G is defined as $L(G) = D(G) - A(G)$.

Distance is an important quantity in graph theory (see [4]). On the one hand, this parameter affects the structure properties and algebraic properties of graphs; on the other hand, this parameter derives some other important distance-based parameters, such as average distance, diameter, radius, eccentricity, distance matrix, resistance distance, and so on, see [18,26,31]. One famous distance-based parameter called the *Wiener index*, $W(G)$, was given by $W(G) = \sum_{i<j} d_{ij}$ in [33], where d_{ij} is the length of a shortest path connecting vertices v_i and v_j in G. For some conclusions and applications, one may be referred to [14,15]. The *Gutman index* of G, was defined as $\mathrm{Gut}(G) = \sum_{i<j} d_i d_j d_{ij}$ by Gutman in [19]. He also showed that when G is a tree of order n, the Wiener index and Gutman index are closely related by $\mathrm{Gut}(G) = 4W(G) - (2n-1)(n-1)$.

On the basis of electrical network theory, Klein and Randić [25] proposed a novel distance function, namely the *resistance distance*, on a graph. The term resistance distance was used because of the physical interpretation: place unit resistors on each edge of a graph G and take the resistance distance, r_{ij}, between vertices v_i and v_j of G to be the effective resistance between them. This novel parameter is in fact intrinsic to the graph and has some nice interpretations and applications in

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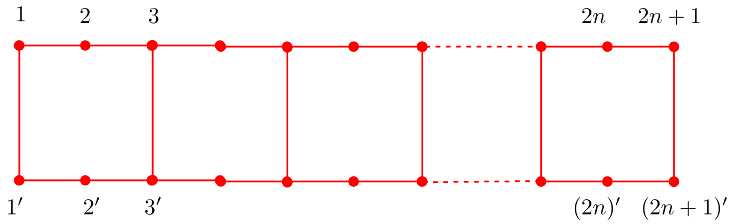

Fig. 1. The linear hexagonal chain L_n with some labeled vertices.

chemistry (see [23,24] for details). As an analogue to the Wiener index, define $K(G) = \sum_{i<j} r_{ij}$, known as the *Kirchhoff index* (a structure-descriptor) of G [25]. Klein and Randić [25] showed that $K(G) \leqslant W(G)$ with equality if and only if G is a tree. For an n-vertex graph G, it is shown, independently, by Klein [24] and Lováz [29] that

$$K(G) = \sum_{i<j} r_{ij} = n \sum_{i=2}^{n} \frac{1}{\mu_i},$$

where $0 = \mu_1 < \mu_2 \leqslant \cdots \leqslant \mu_n$ $(n \geqslant 2)$ are the eigenvalues of $L(G)$.

In recent years, the *normalized Laplacian*, $\mathcal{L}(G)$, which is consistent with the matrix in spectral geometry and random walks [13], has attracted more and more researchers' attention. One of the original motivations for defining the normalized Laplacian was to deal more naturally with nonregular graphs. The normalized Laplacian is defined to be

$$\mathcal{L} = I - D^{\frac{1}{2}}(D^{-1}A)D^{-\frac{1}{2}} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}}$$

(with the convention that if the degree of vertex v_i in G is 0, then $(d_i)^{-\frac{1}{2}} = 0$, see [13]). Thus it is easy to obtain that

$$(\mathcal{L}(G))_{ij} = \begin{cases} 1, & \text{if } i = j; \\ -\dfrac{1}{\sqrt{d_i d_j}}, & \text{if } i \neq j \text{ and } v_i \text{ is adjacent to } v_j; \\ 0, & \text{otherwise,} \end{cases} \tag{1.1}$$

where $(\mathcal{L}(G))_{ij}$ denotes the (i, j)-entry of $\mathcal{L}(G)$. Chen and Zhang [12] showed that the resistance distance can be expressed naturally in terms of the eigenvalues and eigenvectors of the normalized Laplacian and proposed another graph invariant, defined by $K'(G) = \sum_{i<j} d_i d_j r_{ij}$, which is called the *degree-Kirchhoff index* (see [17,21]). It is interesting to see that this novel graph invariant is closely related to the corresponding spectrum of the normalized Laplacian (see Lemma 2.2 in the next section). The spectrum of $\mathcal{L}(G)$ is denoted by $S(G) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ with $0 = \lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_n$. It is well known that G is connected if and only if $\lambda_2 > 0$. After mid 1990s, only a few people devoted to the study of the normalized Laplacian. One may be referred to those in [5,6,9–11].

A hexagonal system (benzenoid hydrocarbon) is a 2-connected plan graph such that each of its interior face (or say a cell) is surrounded by a regular hexagon of unit length one. Let L_n denote a linear hexagonal chain with n hexagons as depicted in Fig. 1. Then it is routine to check that $|V_{L_n}| = 4n+2$ and $|E_{L_n}| = 5n+1$. Hexagonal systems are very important in theoretical chemistry because they are natural graph representations of benzenoid hydrocarbon [20]. Hence, hexagonal systems have been of great interest and extensively studied. In 1991, Kennedy and Quintas [22] considered the prefect matchings in random hexagonal chain graphs. Later, the Wiener index and the Edge-Szeged index of a hexagonal chain are, respectively, determined in [16] and [32]. Recently, Lou and Huang [27] provided a complete description of the characteristic polynomial of a hexagonal system. Yang and Zhang [35] computed the Kirchhoff index of a linear hexagonal chain. For more results on hexagonal system one may be referred to [1,28,30,34–36] and the references therein.

In this paper, inspired by [12,21,27,35], we obtained the decomposition theorem for the normalized Laplacian polynomial. Based on this result, explicit formulas for the degree-Kirchhoff index and the number of spanning trees of L_n are determined, respectively. Moreover, we are surprised to see that the degree-Kirchhoff index of L_n is approximately one half of its Gutman index.

2. Normalized Laplacian polynomial decomposition and some preliminary results

Throughout this paper, we shall denote by $\Phi(B) = \det(xI - B)$ the *characteristic polynomial* of the square matrix B. In particular, if $B = \mathcal{L}(G)$, we write $\Phi(\mathcal{L}(G))$ by $\Psi(G; x)$ and call $\Psi(G; x)$ the *normalized Laplacian characteristic polynomial* of G.

An *automorphism* of G is a permutation π of V_G, which has the property that uv is an edge of G if and only if $\pi(u)\pi(v)$ is an edge of G.

Suppose that G has an automorphism π, which can be written as the product of disjoint 1-cycles and transpositions, that is

$$\pi = (\bar{1})(\bar{2})\cdots(\bar{m})(1, 1')(2, 2')\cdots(k, k').$$