Eigenvector and Eigenvalues of Some Special Graphs. IV. Multilevel Circulants

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Abstract

A multilevel circulant is defined as a graph whose adjacency matrix has a certain block decomposition into circulant matrices. A general algebraic method for finding the eigenvectors and the eigenvalues of multilevel circulants is given. Several classes of graphs, including regular polyhedra, suns, and cylinders can be analyzed using this scheme.

1. Introduction

The last two decades have seen a growing interest in the applications of graph theory to the analysis of chemical graphs [1–11]. Applications of graph theory to molecular orbital theory have been described by Gutman and Polansky [12], by Kiang [13], and by Dias [14]. Most efforts in this field have concentrated on eigenvalues; only a very few papers addressed finding the eigenvectors [2,14]. Some fundamental work concerning the internal connectivity of molecular orbital graphs [15] is also related. It would be helpful if we were able to find the eigenvectors and eigenvalues of graphs without complicated calculations. In this paper, we give an application of an algebraic method for such calculations to chemical graph theory.

Recently, we gave a method [16] for finding eigenvectors and eigenvalues of some special graphs that are well studied in chemistry using linear algebraic methods. The essence of this strategy is to describe the graph in terms of typical operations on subgraphs, such as products and sums. Then, the eigenvectors and eigenvalues of the large graph can be computed from those of its subgraphs. This strategy was successfully applied to the class of hypercubes [17]. These graphs are direct products of complete graphs of order 2, K_2, which is isomorphic to hydrogen-depleted ethene. Linear and cyclic polyenes, whose eigenvectors and eigenvalues can be fully described [18], were used as the starting point in applying this method to graphs such as steps, ladders, cylinders, grids [19], and the class of regular polyhera [20]. Other techniques such as graph splitting were also

developed for similar purposes by Davidson [21], McClelland [22], King [23], and D'Amato [24] and, more recently, by Shen [25].

Circulant graphs have also received some attention [26]. Based on properties of circulants, we formulate a general theorem for obtaining eigenvectors and eigenvalues of multilevel circulants. Then, a number of chemical graphs turn out to be l-level circulants. Thus, their eigenvectors and eigenvalues can be determined.

This paper is structured as follows: A brief review of circulant matrices and the essence of our method is given in Section 2. A detailed description will be published elsewhere [16]. A general theorem concerning multilevel circulants is given in Section 2. Applications of this method to several classes of graphs such as suns, cylinders, and regular polyhera are given in Section 3. Conclusions are drawn in Section 4.

2. The Method

The central theme of this strategy is to construct the eigenvectors and eigenvalues of various graphs that can be defined by algebraic operations, (e.g. direct product) on certain graphs whose eigenvectors and eigenvalues are well known. For a detailed description of this method, one should refer to [16]. Only an outline is stated here.

Let us start with the class of cyclic graphs. They are isomorphic to hydrogendepleted cyclic polyenes, whose eigenvectors and eigenvalues are well known [18]. The adjacency matrix of an n-cycle, C_n, is given by

$$A(C_n) = \begin{bmatrix} 0 & 1 & 0 & \ldots & 0 & 0 \\ 1 & 0 & 1 & \ldots & 0 & 0 \\ 0 & 1 & 0 & \ldots & 0 & 0 \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot \\ 0 & 0 & 0 & \ldots & 0 & 1 \\ 1 & 0 & 0 & \ldots & 1 & 0 \end{bmatrix}.$$

Note that each row is a cyclic permutation of the first row. A square matrix having this property is called a *circulant matrix* or a *circulant*. Thus,

$$A = \begin{bmatrix} a_1 & a_2 & a_3 & \ldots & a_n \\ a_n & a_1 & a_2 & \ldots & a_{n-1} \\ a_{n-1} & a_n & a_1 & \ldots & a_{n-2} \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ a_2 & a_3 & a_4 & \ldots & a_1 \end{bmatrix} \tag{1}$$

is a circulant, denoted $[[a_1, a_2, \ldots, a_n]]$. To describe the eigenvectors and eigenvalues of a circulant, let

$$x = e^{2\pi i/n}.$$

Theorem 0 [27].   A complete set of eigenvectors for $A = [[a_1, a_2, \ldots, a_n]]$ is

$$V_k = (1, x^k, x^{2k}, \ldots, x^{(n-1)k})^t, \tag{2}$$

where $k = 0, 1, 2, \ldots, (n - 1)$ and t denotes transposition. The eigenvalue corresponding to V_k is

$$\lambda_k = \sum_i a_i x^{(i-1)k}. \tag{3}$$

So, for the cycle, the kth eigenvector of $A(C_n)$ is given by (2) with corresponding eigenvalue $\lambda_k = 2 \cos(2k\pi/n)$. This result was obtained by Coulson and Streitwieser [18] using a different method.

A short remark should be made about the relation of the spectrum of a graph to its labeling. Different label assignments would certainly produce different adjacency matrices. If A_1 and A_2 are adjacency matrices that arise from two different labelings of the same graph, then $A_1 = P^{-1}A_2P$ for some permutation matrix P. But the spectrum of a matrix A is the same as that of $B^{-1}AB$, where B is any nonsingular matrix [27], so the spectrum of a graph is invariant with respect to the labeling of the graph.

The *step* or *circulant graphs* are a class of graphs whose matrices are circulants. Let the vertices of our graph be labeled $v_1, \ldots, v_n$. A *step graph*, $C_n(\{n_i\}) = C_n(n_1, n_2, \ldots, n_p)$, where $1 \leq n_1 < n_2 < \ldots < n_p \leq n/2$, is created by making vertex v_i adjacent to each vertex v_k where $k \equiv i + n_j \pmod{n}$ for some n_j. The integers n_j are called the *jump sizes*. As before, (2) gives the eigenvectors with eigenvalues

$$\lambda_k = 2 \sum_{1 \leq i \leq p} \cos(2n_i \pi k/n) \qquad \text{if } n_p \neq n/2 \tag{4a}$$

or

$$\lambda_k = (-1)^k + 2 \sum_{1 \leq i < p} \cos(2n_i \pi k/n) \qquad \text{if } n_p = n/2. \tag{4b}$$

Note that cycles are just step graphs with a single jump size of 1. Complete graphs, denoted K_n, are also special cases of step graphs with multiple jump sizes ranging from 1 to $[(n - 1)/2]$, where $[(n - 1)/2]$ is the greatest integer not exceeding $(n - 1)/2$. The kth eigenvalue of K_n is

$$\lambda_k = \begin{cases} n - 1 & \text{if } k = 0 \\ -1 & \text{if } k \neq 0, \end{cases} \tag{5}$$

where the eigenvalue -1 has multiplicity $n - 1$.

Algebraic operations on graphs such as Cartesian product, Kronecker product, and direct sum can be used to generate new graphs from parent graphs. The key feature of the adjacency matrices of the derived graphs is a 2×2 block form where the diagonal blocks describe the edges among vertices of each parent graph and the off-diagonal blocks record the edges between two of the parents (see [17, 19, 20] for examples). The idea can be easily extended to graphs whose adjacency matrices can be expressed in $l \times l$ block form. We next state a general theorem concerning the eigenvectors and the eigenvalues of such matrices [16]. We will use the following notation: If $A = [a_{ij}]$ and B are matrices of dimensions

$n \times m$ and $n' \times m'$, respectively, then their *tensor product* is the $nn' \times mm'$ matrix with block form

$$A \otimes B = [a_{ij}B].$$

Theorem 1. Let A_{ij}, $1 \le i, j \le l$, be square matrices of order n that have the same complete set of eigenvectors $\{V_1, V_2, \ldots, V_n\}$ with

$$A_{ij} V_k = \alpha_{ij}^{(k)} V_k.$$

Let $B_k = [\alpha_{ij}^{(k)}]$, $1 \le k \le n$, be square matrices of order l, each with a complete set of eigenvectors $\{U_1^{(k)}, U_2^{(k)}, \ldots, U_l^{(k)}\}$ satisfying

$$B_k U_j^{(k)} = \beta_j^{(k)} U_j^{(k)}$$

for $1 \le j \le l$. Then, a complete set of eigenvectors $\{W_1, W_2, \ldots, W_{nl}\}$ for the square matrix

$$A = \begin{bmatrix} A_{11} & A_{12} & \ldots & A_{1l} \\ A_{21} & A_{22} & \ldots & A_{2l} \\ \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \\ \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \\ A_{l1} & A_{l2} & \ldots & A_{ll} \end{bmatrix} \tag{6}$$

is given by

$$W_{(k-1)l+j} = U_j^{(k)} \otimes V_k$$

for $k = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, l$. The corresponding eigenvalues are

$$\lambda_{(k-1)l+j} = \beta_j^{(k)}.$$

We will apply this theorem to the case where all blocks in the adjacency matrix are circulant matrices. An *l-level circulant graph* is one whose adjacency matrix has an $l \times l$ block form (6), all A_{ij} being circulants. For example, a 2-level circulant,

$$G = C_n(\{n_i^{(1)}\}, \{n_i^{(2)}\}; \{m_i^{(12)}\}),$$

would consist of two vertex sets $S_1 = \{v_1, \ldots, v_n\}$ and $S_2 = \{w_1, \ldots, w_n\}$ such that

(a) G induces circulants $C_n(\{n_i^{(1)}\})$ and $C_n(\{n_i^{(2)}\})$ on S_l and S_2, respectively.
(b) Edges between the two circulants are of the form $v_j w_k$, where

$$k = j + m_i^{(12)}(\bmod n)$$

  for some i.

Thus,

$$A(C_n(\{n_i^{(1)}\}, n_i^{(2)}\}; \{m_i^{(12)}\})) = \begin{bmatrix} A(C_n(\{n_i^{(1)}\})) & B \\ B^T & A(C_n(\{n_i^{(2)}\})) \end{bmatrix}, \tag{6a}$$

where $B = [[a_1, a_2, \ldots, a_n]]$ with

$$a_k = \begin{cases} 1 & \text{if } k = 1 + m_i^{(12)}(\bmod n) \text{ for some } i \\ 0 & \text{otherwise.} \end{cases}$$

Suppose α_k and δ_k are the eigenvalues of $A(C_n\{n_i^{(1)}\})$ and $A(C_n\{n_i^{(2)}\})$, respectively, corresponding to the eigenvector V_k of (2). Then, a complete set of eigenvectors for $C_n(\{n_i^{(1)}\},\{n_i^{(2)}\}; \{m_i^{(12)}\})$ is given by

$$\{W_{2k-1}, W_{2k}\} = \left\{ \begin{bmatrix} V_k \\ \alpha V_k \end{bmatrix} : \beta_k \alpha^2 + (\alpha_k - \delta_k)\alpha - \lambda_k = 0 \right\},$$

where

$$\beta_k = \sum_i a_i x^{(i-1)k}$$

$$\gamma_k = \sum_i a_i x^{(n+1-i)k}$$

provided that $\beta_k \neq 0$. The corresponding eigenvalues are

$$\{\lambda_{2k-1}, \lambda_{2k}\} = \{\alpha_k + \beta_k\alpha : \beta_k\alpha^2 + (\alpha_k - \delta_k)\alpha - \gamma_k = 0\}.$$

An l-level circulant is denoted as

$$C(\{n_i^{(1)}\},\{n_i^{(2)}\},\ldots,\{n_i^{(l)}\}; \{m_i^{(12)}\},\{m_i^{(13)}\},\ldots,\{m_i^{(l-1l)}\}),$$

where the $n_i^{(k)}$'s stand for intracirculant jump sizes in the kth circulant and the $m_i^{(hk)}$ stand for intercirculant jump sizes between the hth and kth circulants. Several classes of graphs such as regular polyhedra, suns, and cylinders are used as examples in the next section.

3. Examples

Special Circulants

Matrices of all zeros or all ones, denoted by 0 and J, respectively, are circulant matrices. The identity matrix I is also a circulant. A zero matrix is the adjacency matrix of the graph consisting of n isolated points. All-one matrices and identity matrices do not correspond to adjacency matrices of any chemical graphs, but can represent the coupling between two subgraphs as we will see below. Another circulant matrix is $B = J - I$. It can be viewed as the adjacency matrix of a complete graph or a coupling matrix.
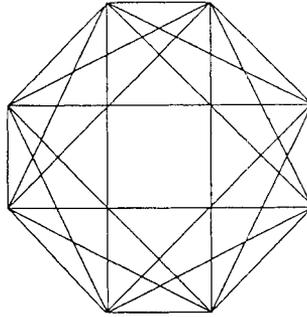
1-Level Circulants

1-level circulants are the simplest circulant graphs. Well-known chemical graphs whose adjacency matrices belong to this class are n-cycles and complete graphs. The eigenvectors and eigenvalues of a 1-level circulant are given in Eqs. (2), (4a), and (4b). For cycles, one can also find them in the *handbook of electronic structures of conjugated systems* [18]. A 1-level circulant may have multiple jump sizes, and two examples are given in Figures 1–2.

$$C_8(\{1, \ 3\})$$

Figure 1.

$$C_8(\{1, \ 2, \ 5\})$$

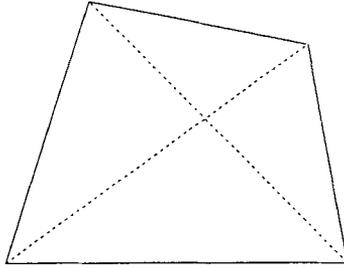Figure 2.

2-Level Circulants

Two K_2's can be coupled by an identity matrix to form a 4-cycle, $C_2(\{1\},\{1\}; \{0\})$, whose adjacency matrix can be written as

$$\begin{bmatrix} A(K_2) & I \\ I & A(K_2) \end{bmatrix}. \tag{7}$$

Alternatively, they can be coupled by a matrix of ones to form a tetrahedron as in Figure 3. This graph is denoted $C_2(\{1\},\{1\}; \{0,1\})$ with adjacency matrix
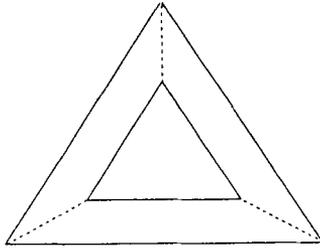
$$\begin{bmatrix} A(K_2) & J \\ J & A(K_2) \end{bmatrix}. \tag{8}$$

Two 3-cycles can be coupled by the identity I or by B, which results in a triangular prism or octahedron, respectively (see Figs. 4 and 5). These graphs are

$$C_2(\{1\},\{1\};\{0,1\})$$

Figure 3.

$$C_3(\{1\},\{1\};\{0\})$$

Figure 4.
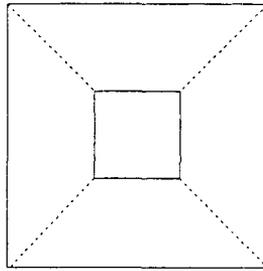
$$C_3(\{1\},\{1\};\{0,1\})$$

Figure 5.

$C_3(\{1\},\{1\}; \{0\})$, and $C_3(\{1\}, \{1\}; \{0, 1\})$, respectively, and have adjacency matrices

$$\begin{bmatrix} A(C_3) & I \\ I & A(C_3) \end{bmatrix} \quad \begin{bmatrix} A(C_3) & B \\ B & A(C_3) \end{bmatrix}. \tag{9}$$

Similarly, $C_4(\{1\},\{1\}; \{0\})$ represents the cube in Figure 6. The famous Petersen graph [28] is a 2-level circulant built up from two 5-cycles, denoted $C_5(\{1\},\{2\}; \{0\})$. Suns and flag-stars are also 2-level circulants of the form $C_n(\{0\},\{1\}; \{0\})$ and $C_n(\{0\},\{1\}; \{0,1\})$ (see Figs. 7 and 8).
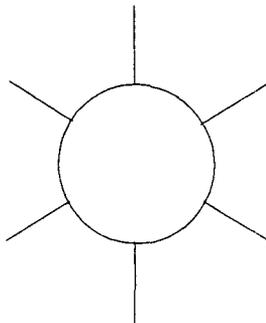
Multilevel Circulants

Buckminsterfullerene C_{60} can be classified as a 12-level circulant. Labeling its vertices as in Figure 9 and then listing them in the order $1, 2, \ldots, 30, 30', \ldots,$
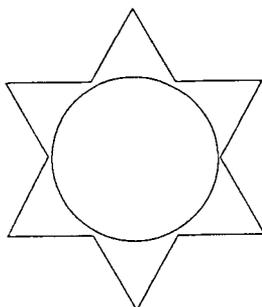

$$C_4 \left(\{1\}, \{1\}; \{0\} \right)$$

Figure 6.

$$C_6 \left(\{0\}, \{1\}; \{0\} \right)$$

Figure 7.

$$C_6\left(\{0\},\{1\};\{0,1\}\right)$$

Figure 8.

$2', 1'$, we obtain the adjacency matrix

$$\begin{bmatrix}
A(C_5) & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
I & 0 & I & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & I & 0 & K^t & 0 & I & 0 & 0 & 0 & 0 & 0 \\
0 & I & K & 0 & I & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & I & 0 & I & L^t & 0 & 0 & 0 & 0 \\
0 & 0 & I & 0 & I & 0 & 0 & L & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & L & 0 & 0 & I & 0 & I & 0 \\
0 & 0 & 0 & 0 & 0 & L^t & I & 0 & I & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & K & I \\
0 & 0 & 0 & 0 & 0 & 0 & I & 0 & K^t & 0 & I \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I & I & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I
\end{bmatrix}, \qquad (10)$$

where each block is 5×5 and

$$K = [[0,1,0,0,0,0]], \qquad L = [[0,0,1,0,0]].$$

A set of eigenvectors and eigenvalues of C_{60} can now be obtained as a corollary to Theorem 1.

Regular Polyhedra

There are exactly five regular polyhedra: the tetrahedron, cube, octahedron, dodecahedron, and icosahedron. We have already seen how the tetrahedron, cube, and octahedron can be viewed as 2-level circulants. For the case of dodecahedron and icoshedron, we proceed as follows: For convenience, we label the vertices of these two regular polyhedra as shown in Figures 10 and 11. As can be seen from Figure 10, the dodecahedron is divided into two subsets of vertices. Each subset is a circulant of size 10, one with jump size 1 and the other with jump
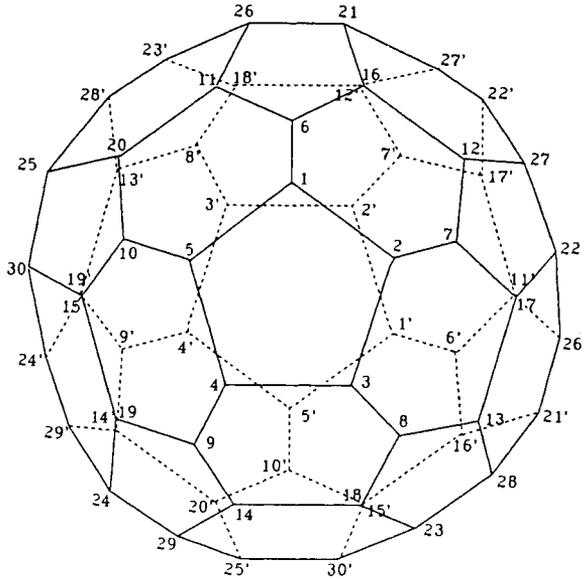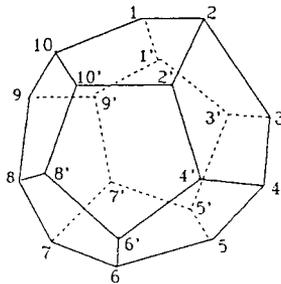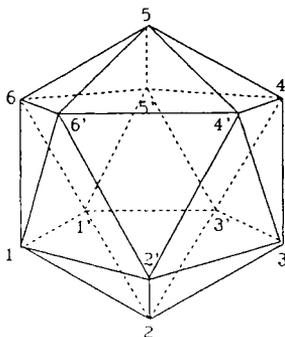
Figure 9.   Labeling of the Buckminsterfullerene C_{60}.

$$C_{10}(\{1\},\{2\};\{0\})$$

Figure 10.

size 2. Listing the vertices in the order $1, 2, \ldots, 10, 1', 2', \ldots, 10'$, we obtain

$$A(\text{dodecahedron}) = \begin{bmatrix} A(C_{10}) & I \\ I & A(C'_{10}) \end{bmatrix}, \tag{11}$$

where $A(C_{10})$ is the central 10-cycle and $C'_{10} = C_{10}(\{2\})$ is composed of the front and rear 5-cycles. Thus, the dodecahedron is a 2-level circulant $C_{10}(\{1\}, \{2\}; \{0\})$. In the case of icosahedron, the system is also divided into two subsets of vertices each having six vertices as shown in Figure 11. Listing the vertices in the order

$$C_6 \left(\{ 1 \}, \{ 2 \}; \{ 0, 1, -1 \} \right)$$

Figure 11.

$1, 2, \ldots, 6, 1', 2', \ldots, 6'$, we obtain

$$A(\text{icosahedron}) = \begin{bmatrix} A(C_6) & M \\ M & A(C_6') \end{bmatrix}, \tag{12}$$

where C_6 is the central 6-cycle, $C_6' = C_6(\{2\})$ is composed of the front and rear 3-cycles, and $M = [[1, 1, 0, 0, 0, 1]]$. Thus the icosahedron is the 2-level circulant $C_6(\{1\}, \{2\}; \{0, 1, -1\})$.

4. Conclusions

We have shown that various graphs used in chemistry can be described as circulants. These include cycles, suns, flag-stars, prisms, the regular polyhedra, and Buckminsterfullerene C_{60}. The eigenvectors and eigenvalues of these graphs can now be calculated using Theorem 1.

Acknowledgment

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