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ON THE ENERGY AND SPECTRAL PROPERTIES OF THE HE MATRIX OF HEXAGONAL SYSTEMS

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Abstract. The He matrix, put forward by He and He in 1989, is designed as a means for uniquely representing the structure of a hexagonal system (= benzenoid graph). Observing that the He matrix is just the adjacency matrix of a pertinently weighted inner dual of the respective hexagonal system, we establish a number of its spectral properties. Afterwards, we discuss the number of eigenvalues equal to zero of the He matrix of a hexagonal system. Moreover, we obtain a relation between the number of triangles and the eigenvalues of the He matrix of a hexagonal system. Finally, we present an upper bound on the He energy of hexagonal systems.

Keywords: molecular graph, hexagonal system, inner dual, He matrix, spectral radius, eigenvalue, energy of graph

MSC 2010: 05C30, 68R10, 81Q30, 05C10

1. Introduction

A hexagonal system can be viewed as a planar arrangement of mutually congruent (connected or disconnected) regular hexagons. For a detailed treatment of hexagonal systems, we refer to [1], [2], [6]. Apart from their various applications in telecommunications, hexagonal systems are of great significance in chemistry structures (see [6] and some references therein).

A technique to reduce the number of vertices and edges in our graphical model of hexagons is to construct the inner dual graph of the hexagonal system. This is constructed by replacing each hexagon with a vertex, and joining two vertices with

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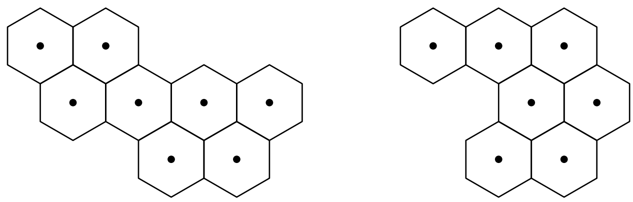
an edge if their corresponding hexagons are adjacent. In the following, we discuss the details of the inner dual of hexagonal systems.

The most common algebraic representation of a graph is the adjacency matrix, followed by the Laplacian matrix, incidence matrix and various other forms [3], [4]. While capturing most structural information of graphs, these matrices ignore the orientation of edges in the graph. Generally, graphs do not have edges in particular directions/orientations, so it is not necessary to represent it. However, in the case of hexagonal systems, a given hexagon can have another hexagon adjacent to it only from 6 directions (i.e., from each side). Thus two hexagons can only be connected at $0°$, $60°$ or $120°$ relative to the horizontal axis. For this reason, we use the He matrix, which records the orientation of edges in the inner dual graph. For more details on the He matrix see [6].

For the inner dual, we follow the description given in [6]. Consider the examples shown in Figure 1.

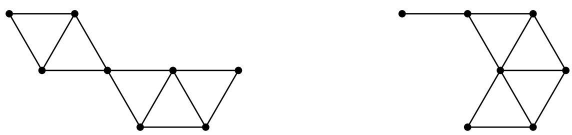


(a) Graph H_1 (b) Graph H_2

Figure 1. Two hexagonal systems. Their inner duals are shown in Figure 2.

Definition 1.1. The inner dual ID(H) of a hexagonal system H is a graph constructed by placing a vertex in the center of each hexagon of H and connecting those vertices that are in adjacent hexagons.

In Figure 2, we show the inner duals of the hexagonal systems in Figure 1.



(c) Graph ID(H_1) (d) Graph ID(H_2)

Figure 2. The inner duals ID(H_1) and ID(H_2) of the hexagonal systems H_1 and H_2 in Figure 1.

While [6] mainly discusses the spectral properties of the inner dual of a hexagonal system using the He matrix, in this paper we establish relationships between some spectral and structural properties.

The elementary spectral properties of the He matrix have been studied in [6]. In [6], it has been defined that the He energy is the sum of the absolute values of the eigenvalues of the He matrix of a hexagonal system. The He energy is different from other energies, i.e., adjacency, Laplacian [8], etc., which have been studied extensively in the literature. The rest of the paper is organized as follows. In Section 2, we determine the characterization of hexagonal systems from the spectral radius of the He matrix. In Section 3, we discuss the number of eigenvalues equal to zero of the He matrix of a hexagonal system. In Section 4, we obtain a relation between the number of triangles and the eigenvalues of the He matrix of a hexagonal system.

In Section 5 we give our main results on the upper bounds for the He energy in terms of edge orientations. This is followed by the Section 6 on coalescence of hexagonal systems, with the emphasis on the energy of coalesced systems. We also show that to satisfy the inner dualist of coalesced systems, new edges have to be added to the existing system.

Here we give the formal definition of the He matrix:

Definition 1.2. Let H be a hexagonal system with n hexagons. Let the vertices of the dualist graph of H be labeled by $1, 2, \ldots, n$. Denote by (rs) the edge of the dualist graph connecting the vertices r and s. Sometimes, we use the notation $i \sim j$, when vertices i and j are adjacent. Then the He matrix $A(H)$ of H is a square matrix of order n whose (i,j)-entry a_{ij} is defined as follows:

$$a_{ij} = \begin{cases} 0 & \text{if } i = j \text{ or if the vertices } i \text{ and } j \text{ of the dualist graph are not adjacent,} \\ 1 & \text{if } (ij) \text{ is an edge, and the angle between } (ij) \\ & \text{and the horizontal direction is } k\pi, \\ 2 & \text{if } (ij) \text{ is an edge, and the angle between } (ij) \\ & \text{and the horizontal direction is } k\pi + \pi/3, \\ 3 & \text{if } (ij) \text{ is an edge, and the angle between } (ij) \\ & \text{and the horizontal direction is } k\pi + 2\pi/3. \end{cases}$$

Since $A(H)$ is symmetric and real, and all the diagonal elements are zero, the eigenvalues of $A(H)$ are real and their sum is equal to zero. The eigenvalues of $A(H)$ form the spectrum of the He matrix and may be ordered as

$$\lambda_1(A(H)) \geqslant \lambda_2(A(H)) \geqslant \ldots \geqslant \lambda_n(A(H)).$$

In the rest of the paper we will write $\lambda_i(H)$ or simply λ_i instead of $\lambda_i(A(H))$.

2. Characterization of hexagonal systems from the spectral radius of the He matrix

In this section, we determine the characterization of hexagonal systems from the spectral radius of the He matrix. The following is a result of Perron-Frobenius in matrix theory [7], which we need in our paper at a later stage.

Lemma 2.1. *A non-negative matrix B always has a non-negative eigenvalue r such that the moduli of all the eigenvalues of B do not exceed r. To this "maximal" eigenvalue r there corresponds a non-negative eigenvector $\mathbf{Y}$ such that*

$$B\mathbf{Y} = r\mathbf{Y} \quad (\mathbf{Y} \geqslant \mathbf{0}, \mathbf{Y} \neq \mathbf{0}).$$

Lemma 2.2 [9]**.** *Let $B = \|b_{ij}\|$ be an $n \times n$ irreducible non-negative matrix with spectral radius $\lambda_1(B)$, and let $R_i(B)$ be the i-th row sum of B, i.e., $R_i(B) = \sum_{j=1}^{n} b_{ij}$. Then*

$$\min\{R_i(B)\colon\ 1 \leqslant i \leqslant n\} \leqslant \lambda_1(B) \leqslant \max\{R_i(B)\colon\ 1 \leqslant i \leqslant n\}. \tag{2.1}$$

Moreover, if the row sums of B are not all equal, then both inequalities in (2.1) *are strict.*

Lemma 2.3. *Let B be a $p \times p$ symmetric matrix and let B_k be its leading $k \times k$ submatrix; that is, B_k is the matrix obtained from B by deleting its last $p-k$ rows and columns. Then, for $i = 1, 2, \ldots, k$,*

$$\lambda_{p-i+1}(B) \leqslant \lambda_{k-i+1}(B_k) \leqslant \lambda_{k-i+1}(B), \tag{2.2}$$

where $\lambda_i(B)$ is the i-th largest eigenvalue of B.

We now give a lower bound on the spectral radius of the He matrix of a hexagonal system.

Theorem 2.4. *Let H be a hexagonal system with n hexagons. Then the spectral radius of the He matrix is given by*

$$\lambda_1(H) \geqslant \max_i \left\{ \sqrt{\sum_{j\colon\, j\sim i} a_{ij}^2} \right\}. \tag{2.3}$$

P r o o f. Let ID(H) be the dualist graph corresponding to the hexagonal system H. By Lemma 2.3, we have

$$\lambda_1(H) \geqslant \lambda_1(H^*), \tag{2.4}$$

where H^* is the square submatrix $k \times k$ obtained from H by deleting the rows and columns except the i-th and j-th such that $j \sim i$. Let $\mathbf{X} = (x_1, x_2, \ldots, x_k)^T$ be an eigenvector corresponding to the eigenvalue $\lambda_1(H^*)$ of the dualist graph H^*. We can assume that $x_i = \max\limits_j x_j$. Then we have

$$\lambda_1(H^*)x_i = \sum_{j\,:\,j\sim i} a_{ij}x_j,$$

that is,

$$\lambda_1^2(H^*)x_i = \sum_{j\,:\,j\sim i} a_{ij}\lambda_1(H^*)x_j.$$

Since $\lambda_1(H^*)x_j \geqslant a_{ij}x_i$ for all $j \sim i$ (as all $x_t \geqslant 0$, by Lemma 2.1), using (2.4) we get the required result (2.3). □

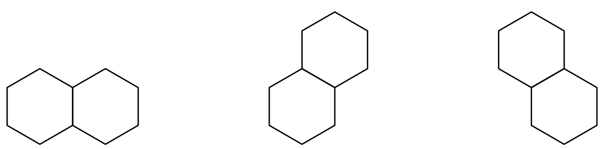
In the following we give the results in the form of corollaries.

Corollary 2.5. *Let* ID(H) *be the dualist graph of* H *with maximum degree 6. Then* $\lambda_1 > 5.29$.

Corollary 2.6. *Let* ID(H) *be the dualist graph of* H *with maximum degree greater than or equal to 5. Then* $\lambda_1 > 4.358$.

Corollary 2.7. *Let* ID(H) *be the dualist graph of* H *with maximum degree greater than or equal to 4. Then* $\lambda_1 > 3.162$.

Let H_3 be a hexagonal system with two hexagons (the "naphthalene graph"), see Figure 3 (obtained from [6]). The spectrum of its He matrix is either $\{-1,1\}$ or $\{-2,2\}$ or $\{-3,3\}$, depending on the way in which H_3 is drawn. Thus the spectrum of $\mathbf{A}(H_3)$ is integral.



H_{3a} H_{3b} H_{3c}

Figure 3. A hexagonal system whose He matrix has integral spectrum. For the orientations H_{3a}, H_{3b}, and H_{3c}, the spectra of $\mathbf{A}(H_3)$ are $\{-1,1\}$, $\{-2,2\}$, and $\{-3,3\}$, respectively.

From the definition, the edges of the dualist graphs have three different possible directions. We classify them into types (a), (b), and (c), so that an edge e is of type

(a) if the angle between e and the positive horizontal direction is either 0 or π,

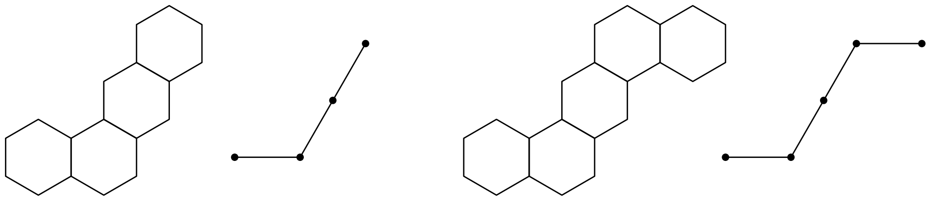
(b) if the angle between e and the positive horizontal direction is either $\pi/3$ or $4\pi/3$, and

(c) if the angle between e and the positive horizontal direction is either $2\pi/3$ or $5\pi/3$.

Now we will determine the characterization of hexagonal systems from the integral spectral radius.

Theorem 2.8. *Let H be a hexagonal system with n hexagons. Also let $\lambda_1(H) = i$ for $i = 1, 2, 3$. Then $H \cong H_{3a}$ or $H \cong H_{3b}$ or $H \cong H_{3c}$ or $H \cong H_5$ (in Figure 4).*

P r o o f. Suppose $\mathrm{ID}(H)$ is the dualist graph corresponding to the hexagonal system H. Using Corollary 2.7, we conclude that the maximum degree of $\mathrm{ID}(H)$ is less than or equal to 3. If $n = 2$, then $\lambda_1 = 1$ and $H \cong H_{3a}$, or $\lambda_1 = 2$ and $H \cong H_{3b}$, or $\lambda_1 = 3$ and $H \cong H_{3c}$. Otherwise, $n \geqslant 3$ and the maximum degree of $\mathrm{ID}(H)$ is 2 or 3. Now we construct a hexagonal system H'_{3c} corresponding to dualist graph $\mathrm{ID}(H'_{3c})$, by adding a pendant edge in any direction to any one vertex in $\mathrm{ID}(H_{3c})$. Then one can see easily that $\lambda_1(H'_{3c}) > 3$ as $n \geqslant 3$. If $\mathrm{ID}(H'_{3c})$ is a subgraph of $\mathrm{ID}(H)$, then $\lambda_1(H) > 3$ and we are done. Otherwise, $\mathrm{ID}(H'_{3c})$ is not a subgraph of $\mathrm{ID}(H)$. From this we conclude that there is no edge of type (c) in $\mathrm{ID}(H)$. If the maximum degree of $\mathrm{ID}(H)$ is 3, then we must have at least one edge of type (c) in $\mathrm{ID}(H)$, which is a contradiction. Otherwise, maximum degree of $\mathrm{ID}(H)$ is 2. First we assume that $\mathrm{ID}(H)$ is isomorphic to a path P_n with all the edges in two different possible directions. When all the edges of the path P_n are of type (a), we have $1 < \lambda_1(H) < 2$. When all the edges of the path P_n are of type (b), we have $3 < \lambda_1(H) < 4$ for $n \geqslant 4$ and $2 < \lambda_1(H) < 3$ for $n = 3$. Next we assume that $\mathrm{ID}(H)$ is isomorphic to a path P_n with the edges of type (a) and (b). From above we have seen that at most two consecutive edges are of type (b) in $\mathrm{ID}(H)$, otherwise $\lambda_1(H) > 3$. If there is one edge of type (b) adjacent to edges of type (a) in the path P_n, then by Lemma 2.2, $2 < \lambda_1(H) < 3$. It remains to show that two consecutive edges are of type (b), adjacent to edges of type (a) in path P_n. So $\mathrm{ID}(H_4)$ or/and $\mathrm{ID}(H_5)$ are subgraphs of $\mathrm{ID}(H)$ (see Figure 4). By Mathematica, we have $\lambda_1(H_5) = 3$. One can see readily that $\lambda_1(H) > 3$ if $\mathrm{ID}(H_5)$ is a strict subgraph of $\mathrm{ID}(H)$. Now we consider the matrix $D^{-1}A(H)D$, where D is the diagonal matrix whose diagonal elements are the degrees of the dualist graph. It is well known that $\lambda_1(D^{-1}A(H)D) = \lambda_1(A(H))$. If $\mathrm{ID}(H_4)$ is a subgraph of $\mathrm{ID}(H)$, but $\mathrm{ID}(H_5)$ is not a subgraph of $\mathrm{ID}(H)$, then $\lambda_1(H) = \lambda_1(D^{-1}A(H)D) < 3$, by Lemma 2.2. This completes the proof. $\square$



H_4 $\qquad$ $\mathrm{ID}(H_4)$ $\qquad$ H_5 $\qquad$ $\mathrm{ID}(H_5)$

Figure 4. Two hexagonal systems H_4, H_5 and their inner duals $\mathrm{ID}(H_4)$, $\mathrm{ID}(H_5)$.

3. Eigenvalues equal to zero in hexagonal system

In this section we discuss the number of eigenvalues equal to zero in a hexagonal system. Let H_0 be a hexagonal system with the corresponding inner dual $\mathrm{ID}(H_0)$. Also let v be vertex of the inner dual $\mathrm{ID}(H_0)$. Construct a hexagonal system H_1 with the corresponding inner dual $\mathrm{ID}(H_1)$ from $\mathrm{ID}(H_0)$ by attaching a new pendant vertex to v such that the angle between the pendant edge and the positive horizontal direction is 0 or $\pi/3$ or $2\pi/3$ or π or $4\pi/3$ or $5\pi/3$. Construct a hexagonal system H_2 with the corresponding inner dual $\mathrm{ID}(H_2)$ by attaching one pendant vertex to v in $\mathrm{ID}(H_1)$ such that the angle between these two pendant edges is $2\pi/3$ or π or $4\pi/3$. If the two pendant vertices are labeled by 1 and 2, and the vertex v by 3, then the He matrix is of the form

$$A(H_2) = \begin{pmatrix} 0 & 0 & a_{13} & 0 & \dots & 0 \\ 0 & 0 & a_{23} & 0 & \dots & 0 \\ a_{13} & a_{23} & * & * & \dots & * \\ 0 & 0 & * & * & \dots & * \\ \cdot & \cdot & \cdot & \cdot & \dots & \cdot \\ 0 & 0 & * & * & \dots & * \end{pmatrix},$$

where $*$ stands for the He matrix of $\mathrm{ID}(H_0)$.

The He characteristic polynomial of an inner dual $\mathrm{ID}(H)$ is defined by $\psi(H) = \psi(H, \lambda) = \det(\lambda I - A(H))$. Then

$$\psi(H_2) = \begin{vmatrix} \lambda & 0 & -a_{13} & 0 & \dots & 0 \\ 0 & \lambda & -a_{23} & 0 & \dots & 0 \\ -a_{13} & -a_{23} & * & * & \dots & * \\ 0 & 0 & * & * & \dots & * \\ \cdot & \cdot & \cdot & \cdot & \dots & \cdot \\ 0 & 0 & * & * & \dots & * \end{vmatrix},$$

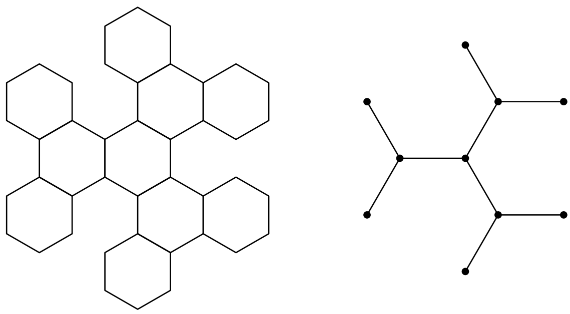
where now $*$ indicates $\psi(H_0, \lambda)$.

By pertinent transformations of the above determinant we arrive at

$$\psi(H_2) = \left(1 + \frac{a_{13}^2}{a_{23}^2}\right)\lambda\psi(H_1) - \lambda^2 \frac{a_{13}}{a_{23}}\,\psi(H_0). \tag{3.1}$$

From (3.1), we obtain the following result:

Theorem 3.1. *Let H be a hexagonal system with the corresponding inner dual* $\mathrm{ID}(H)$. *If any two pendant edges incident to the same vertex with angle $2\pi/3$ or π or $4\pi/3$ in any inner dual* $\mathrm{ID}(H)$, *then 0 is an eigenvalue in H.*



H_6 $\qquad$ $\mathrm{ID}(H_6)$

Figure 5. Hexagonal system H_6, and its inner dual $\mathrm{ID}(H_6)$.

By Theorem 3.1, these are at least three eigenvalues of the He matrix $A(H_6)$ of the hexagonal system H_6 equal to zero. Actual eigenvalues of $A(H_6)$ are $\{4.65224, -4.65224, -3.52922, 3.52922, -2.81092, 2.81092, 0, 0, 0, 0\}$.

4. The number of triangles

It is mentioned in [5] that the number of closed paths of length 3 is equal to the 3-rd spectral moment of the adjacency matrix. Therefore, $\sum_{i=1}^{n} \lambda_{A_i}^3$ is equal to $6 \times \Delta$, where Δ is the number of triangles, λ_{Ai} are the eigenvalues of the adjacency matrix A, and n is the number of vertices.

The motivation for 6 in $6 \times \Delta$ comes from the fact that a triangle of vertices a, b and c can be represented by 6 closed paths of length 3:

$$a{-}b{-}c{-}a, \quad a{-}c{-}b{-}a, \quad b{-}a{-}c{-}b,$$
$$b{-}c{-}a{-}b, \quad c{-}a{-}b{-}c, \quad c{-}b{-}a{-}c.$$

Since $\sum_{i=1}^{n} \lambda_{A_i}^3$ is equal to the number of closed paths of length 3, we get

$$\sum_{i=1}^{n} \lambda_{A_i}^3 = Tr(A^3) = 6 \times \Delta. \tag{4.1}$$

Here we extend the result to the He matrices.

Theorem 4.1. *The number of triangles in a dualist graph of a hexagonal system is related to the cube of the eigenvalues of the He matrix by the equation*

$$\sum_{i=1}^{n} \lambda_i^3 = 36 \times \Delta, \tag{4.2}$$

where Δ *is the number of triangles,* n *is the number of vertices and* λ_i*,* $1 \leqslant i \leqslant n$*, is an eigenvalue of the He matrix.*

Proof. Let A be the adjacency matrix of the dualist graph ID(H). Then

$$\sum_{i=1}^{n} (A^3)_{ii} = \sum_{i=1}^{n}\sum_{p=1}^{n}\sum_{r=1}^{n} a_{ip}a_{pr}a_{ri} \tag{4.3}$$

If there is a closed path i–p–r–i, then this path is a triangle and all of a_{ip}, a_{pr} and a_{ri} will be non-zero and equal to 1.

Now let $A(H)$ be the He matrix, and h_{ij} be the (i, j)-entry in $A(H)$. Then

$$\sum_{i=1}^{n} (A(H)^3)_{ii} = \sum_{i=1}^{n}\sum_{p=1}^{n}\sum_{r=1}^{n} h_{ip}h_{pr}h_{ri}.$$

Due to the restrictions of the He matrix, edges in the triangles will be of orientation $0°$, $60°$ and $120°$, and thus,

$$h_{ip}h_{pr}h_{ri} = \begin{cases} 3 \times 2 \times 1 & \text{(in some order) if the path } i\text{–}p\text{–}r\text{–}i \text{ exists,} \\ 0 & \text{otherwise.} \end{cases}$$

Since

$$a_{ip}a_{pr}a_{ri} = \begin{cases} 1 \times 1 \times 1 & \text{if the path } i\text{–}p\text{–}r\text{–}i \text{ exists,} \\ 0 & \text{otherwise.} \end{cases}$$

We can say that $h_{ip}h_{pr}h_{ri} = 6 \times a_{ip}a_{pr}a_{ri}$ for every i, p, r.

Then,

$$\sum_{i=1}^{n}\sum_{p=1}^{n}\sum_{r=1}^{n} h_{ip}h_{pr}h_{ri} = \sum_{i=1}^{n}\sum_{p=1}^{n}\sum_{r=1}^{n} 6 \times a_{ip}a_{pr}a_{ri},$$

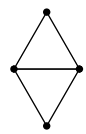
$$\text{i.e.,} \quad \sum_{i=1}^{n}\sum_{p=1}^{n}\sum_{r=1}^{n} h_{ip}h_{pr}h_{ri} = 6 \times \sum_{i=1}^{n}\sum_{p=1}^{n}\sum_{r=1}^{n} a_{ip}a_{pr}a_{ri},$$

$$\text{i.e.,} \quad \sum_{i=1}^{n} (A(H)^3)_{ii} = 6 \times \sum_{i=1}^{n} (A^3)_{ii},$$

$$\text{i.e.,} \quad \sum_{i=1}^{n} {\lambda_i}^3 = 6 \times \sum_{i=1}^{n} \lambda_{Ai}^3 = 36 \times \Delta \text{ by (4.1).}$$

□

For example, consider the following dualist graph ID(H_7):



ID(H_7)

Figure 6. Inner dual ID(H_7) of a hexagonal system H_7.

Let A be the adjacency matrix of ID(H_7), and $A(H_7)$ be the He matrix. Then

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \quad A(H_7) = \begin{pmatrix} 0 & 2 & 3 & 0 \\ 2 & 0 & 1 & 3 \\ 3 & 1 & 0 & 2 \\ 0 & 3 & 2 & 0 \end{pmatrix}$$

Therefore, the eigenvalues of A and $A(H_7)$ are

$$\lambda(A) = \{2.56155, -1.56153, -1, 0\},$$
$$\lambda(A(H_7)) = \{5.52494, -4.52494, -1.61803, 0.618034\},$$

their cubed values are

$$\lambda^3(A) = \{16.8077, -3.8076, -1, 0\},$$
$$\lambda^3(A(H_7)) = \{168.648, -92.6484, -4.23607, 0.236068\},$$

and their 3-rd spectral moments are

$$\sum_{i=1}^{n} \lambda_i^3(A) = 12, \quad \sum_{i=1}^{n} \lambda_i^3(A(H_7)) = 72.$$

Therefore,

$$\sum_{i=1}^{n} \lambda_i^3(A) = 6 \times \Delta, \quad \sum_{i=1}^{n} \lambda_i^3(A(H_7)) = 36 \times \Delta,$$

where Δ is the number of triangles in the inner dual $\mathrm{ID}(H_7)$.

5. Upper bound on the He energy of a hexagonal system

The He energy [6] of a hexagonal system H is defined as $E_H = \sum\limits_{i=1}^{n} |\lambda_i|$, where λ_i, $1 \leqslant i \leqslant n$ are the eigenvalues of the He matrix of the dualist graph $\mathrm{ID}(H)$, and n, and is the number of vertices in $\mathrm{ID}(H)$.

In this section we describe a new relation between the He energy of a dualist graph, the number of vertices n, and the number of edges of each orientation in $\mathrm{ID}(H)$.

For the following theorem and its proof, we define "orientation of the edge (ij)" as the entry in the He matrix at the position (ij). Thus an edge with an orientation of x is at an angle $(x-1) \times 60^\circ$, $x = 1, 2, 3$.

Theorem 5.1. *The He energy E_H of the dualist graph $\mathrm{ID}(H)$ of a hexagonal system H is bounded above by the inequality*

$$E_H \leqslant \sqrt{2n(m_1 + 4m_2 + 9m_3)},$$

where m_i is the number of edges of orientation i, for $1 \leqslant i \leqslant 3$, and n is the number of vertices in $\mathrm{ID}(H)$.

P r o o f. A following well-known relation between the eigenvalues of an $n \times n$ Hermitian matrix $B = (b_{ij})$ and n is

$$\sum_{i=1}^{n} |\lambda_i| \leqslant \sqrt{n} \cdot \|B\|_F, \tag{5.1}$$

where $\|B\|_F$ is the Frobenius norm of B, given by

$$\|B\|_F = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} |b_{ij}|^2}.$$

Now let $A(H)$ be the He matrix of the dualist graph $\mathrm{ID}(H)$ of a hexagonal system H. Thus $a_{ij} = 0$, 1, 2 or 3 for $1 \leqslant i, j \leqslant n$.

We define π_k as the number of entries in $A(H)$ of value k, $0 \leqslant k \leqslant 3$. Thus π_1 is the number of 1's in $A(H)$, and so on. If $A(H) = [a_{ij}]$, squaring the entries in $A(H)$

results in the matrix $A(H^*) = [a_{ij}^2]$. The number of each k^2 $(k = 0, 1, 2, 3)$ in $A(H^*)$ is equal to the number of k's in $A(H)$, i.e.,

$$\# \text{ of } k^2\text{'s in } A(H^*) = \# \text{ of } k\text{'s in } A(H) = \pi_k$$

When adding the entries in $A(H^*)$, all occurrences of k^2 for each k (i.e. occurrences of 0, 1, 4, and 9 in $A(H^*)$) can be grouped. Since π_k represents the number of times each value occurs in $A(H^*)$, this results in:

$$\sum_{i=1}^{n}\sum_{j=1}^{n} |a_{ij}|^2 = \sum_{k=0}^{3} k^2 \pi_k$$

Since each edge is represented by 2 entries in $A(H)$, we have $\pi_k = 2m_k$, where m_k is the number of edges of orientation k. Therefore,

$$\begin{aligned}\sum_{i=1}^{n}\sum_{j=1}^{n} |a_{ij}|^2 = \sum_{k=0}^{3} k^2 \times 2m_k &= 1(2m_1) + 4(2m_2) + 9(2m_3) \\ &= 2(m_1 + 4m_2 + 9m_3).\end{aligned}$$

The Frobenius norm can now be written for the dualist graph of a hexagonal system as

$$\|A(H)\|_F = \sqrt{2(m_1 + 4m_2 + 9m_3)}.$$

From (5.1), we have

$$\sum_{i=1}^{n} |\lambda_i| \leqslant \sqrt{n} \times \sqrt{2(m_1 + 4m_2 + 9m_3)}.$$

Hence the theorem. □

For example, consider the dualist graphs $\mathrm{ID}(H_8)$ and $\mathrm{ID}(H_9)$:

$$\begin{aligned}&\mathrm{ID}(H_8):\ n = 5,\ m_1 = 3,\ m_2 = 2,\ m_3 = 1,\\ &\mathrm{ID}(H_9):\ n = 7,\ m_1 = 3,\ m_2 = 3,\ m_3 = 3\end{aligned}$$

Figure 7. Graph $\mathrm{ID}(H_8)$ with 5 vertices and 6 edges, and graph $\mathrm{ID}(H_9)$ with 7 vertices and 9 edges.

For the dualist graph ID(H_8),

$$A(H_8) = \begin{pmatrix} 0 & 1 & 0 & 2 & 3 \\ 1 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 1 & 0 \\ 2 & 0 & 1 & 0 & 1 \\ 3 & 2 & 0 & 1 & 0 \end{pmatrix},$$

The eigenvalues of $A(H_8)$ are $\{4.88335, -3.31712, -2.04794, 0.888729, -0.40702\}$, and thus the $Energy = E_{H_8} = 11.5442$.

Here,

$$\pi_1 = 6,\ \pi_2 = 4,\ \pi_3 = 2 \quad \Rightarrow \quad m_1 = 3,\ m_2 = 2,\ m_3 = 1$$

and $n = 5$. Thus $\sqrt{2n(m_1 + 4m_2 + 9m_3)} = 10\sqrt{2} \approx 14.142$, which is greater than the energy calculated.

For the dualist graph ID(H_9),

$$A(H_9) = \begin{pmatrix} 0 & 0 & 2 & 3 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 3 & 0 \\ 2 & 1 & 0 & 1 & 0 & 2 & 0 \\ 3 & 0 & 1 & 0 & 1 & 0 & 3 \\ 0 & 0 & 0 & 1 & 0 & 0 & 2 \\ 0 & 3 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 2 & 0 & 0 \end{pmatrix}$$

The eigenvalues of $A(H_9)$ are $\{5.55993, -4.29929, 3.90212, -3.30324, -2.09694, 1.53998, -1.30256\}$, and thus the Energy $= E_{H_9} = 22.0041$.

Now $m_1 = 3$, $m_2 = 3$, $m_3 = 3$, and $n = 5$. Thus $\sqrt{2n(m_1 + 4m_2 + 9m_3)} = 6\sqrt{14} \approx 22.45$, which is greater than the energy calculated.

6. Coalescence

In [11], W. So et al. have described the coalescence of two graphs. The concept can be extended to hexagonal systems. The coalescence of two hexagonal systems can be interpreted as the coalescence of two faces, or hexagons, of each system, which implies a coalescence of the inner dual graphs.

Definition 6.1. Let H_{10} and H_{11} be the inner dual graphs of two hexagonal systems with disjoint vertex sets. Let $u \in H_{10}$ and $v \in H_{11}$. Create a new graph H_{12} by identifying vertices u and v, and call this new vertex w. If $I(x)$ be the set of edges incident on vertex x, $I(w) = I(u) \cup I(v)$. Then H_{12} is called the coalescence of H_{10} and H_{11}.

A simple example is in Figure 8. Vertices u in H_{10} and v in H_{11} are merged to form the inner dual graph H_{12}. The vertices u and v are consolidated into w.

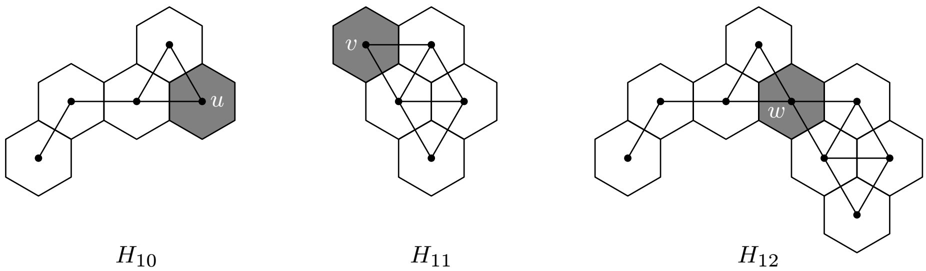


Figure 8. Graphs H_{10}, H_{11} and H_{12}.

The coalescence of hexagonal systems G and H may yield an inner dual graph which is different from simply coalescing the two inner dual graphs of G and H. This is due to two or more hexagons from G and H now becoming adjacent to each other, thereby requiring an additional edge in the new inner dual graph. We call such an edge an induced edge. For example,

Figure 9 (a) and (b) show two graphs that are coalesced on vertices a in H_{13} and d in H_{14}. The vertices a and d merge to form f. Figure 9 (c) shows the coalescence of the hexagonal systems H_{13} and H_{14}, and Figure 9 (d) shows the coalescence of inner dual graphs of H_{13} and H_{14}.

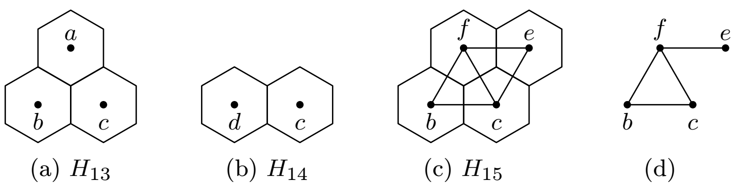


Figure 9. Graphs H_{13}, H_{14} and H_{15}.

The inner dual graph in (d) lacks the edge between hexagons e and c. The edge, however, is present in (c). Therefore the edge (ce) is an induced edge, or in other words, (ce) was induced in the coalescence.

Lemma 6.2. *An edge is induced in the coalescence of G and H wherever an edge from* $\mathrm{ID}(H)$ *makes an angle of* $\pi/3$ *with an edge from* $\mathrm{ID}(G)$.

P r o o f. Since there are 2 edges, there must be 3 vertices/hexagons. If hexagon a is adjacent to c and b is also adjacent to c such that the angle between ac and bc is $\pi/3$, hexagon a must be adjacent to hexagon b. Thus the edge ab must be induced. □

W. So et al. [11] have provided an upper bound on the energy of $G \circ H$. We show that the bound holds when there are no induced edges in $G \circ H$, but in the case of induced edges, the bound increases by the energy of the induced edges.

Hereafter, $E(G)$ stands for the energy of the inner dual graph G, which is defined in [6].

Lemma 6.3. *Let G and H be two hexagonal systems. If there are no induced edges in $G \circ H$, then $E(G \circ H) \leqslant E(G) + E(H)$.*

P r o o f. Since no induced edges are added, the concept remains the same as described in [11]. The proof follows directly from the paper. It should be noted that the method employed in [11] is applicable to all real symmetric matrices, and is thus suitable for the He matrix. □

When there are one or more induced edges, the above result fails in most cases. To this end, we provide the following more general theorem:

Theorem 6.4. *Let G_1 and G_2 be two hexagonal systems. If there exist induced edges in $G_1 \circ G_2$, then*

$$E(G_1 \circ G_2) \leqslant E(G_1) + E(G_2) + E(I)$$

where E(I) is the combined energy of the induced edges.

P r o o f. Consider the inner dual graphs $\mathrm{ID}(G_1)$ and $\mathrm{ID}(G_2)$. Let G' be the hypothetical coalescence of these two graphs if the induced edges were to be ignored. Then the He matrices can be related by:

$$He(G') = He(G_1) + He(G_2).$$

From [11] it follows that

$$E(G') \leqslant E(G_1) + E(G_2).$$

Now let I be the hypothetical graph comprising only of the induced edges. Denote the actual coalescence graph by $G_1 \circ G_2$. Now $G_1 \circ G_2$, G' and I can be related by:

$$He(G_1 \circ G_2) = He(G') + He(I).$$

Again, from [11],

$$E(G1 \circ G2) \leqslant E(G') + E(I).$$

Using the above two inequalities, we arrive at

$$E(G_1 \circ G_2) \leqslant E(G_1) + E(G_2) + E(I).$$

□

There are several graphs where $E(G_1 \circ G_2) \leqslant E(G_1) + E(G_2)$ holds even if there are induced edges. However, such coalescences are not common.

7. Conclusion

In this paper, we have presented some new avenues which have opened up after the introduction of the He matrix in 1986. The idea of the He matrix had been lying untouched for the last 25 years, and after discussions with various chemists and physicists, we are at a loss as to why further work was not conducted on this topic. The He matrix appears to be useful because rotations and reflections of hexagonal systems result in different eigenvalues and energy. It should be noted that the He matrix of a hexagonal system after a rotation of 180° is only a different permutation of the original He matrix; thus it has the same eigenvalues. A few applications originated in chemistry, particularly for the molecular structures, without the use of the spectrum of the He matrix for hexagonal systems.

We have discussed the work that we have conducted on the relationship between a hexagonal system's eigenvalues and its structural properties. Although closely related to eigenvalues, the concept of He energy appears to be so rich in applications that it deserves special attention. Although our work has been more focused on the bounds on the energy of hexagonal systems, earlier work on adjacency matrices have established relationships between the energy of a graph and its rank, chromatic number, etc.—this needs to be propagated to hexagonal systems using the He matrix.

Finally, there remain several areas to be explored in the study of hexagonal systems using the He matrix, both theoretical and applied. This and earlier papers focused mainly on setting the theoretical basis for future studies in applied fields, such as hydrocarbon chemistry, robotics, self-assembly, telecommunications and antennae.

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