The Characteristic Polynomial of a kind of Hexagonal System and its Application*

Caixia Song, Qiongxiang Huang †

College of Mathematics and Systems Science,

Xinjiang University, Urumqi, Xinjiang 830046, P.R.China

Abstract The hexagonal system considered here , denoted by E_n^2, is formed by $3n$ ($n \geq 2$) hexagons shown in Fig.2(a). In this paper, we give the explicit expression of characteristic polynomial $\Phi_A(E_n^2, x)$. Subsequently, we obtain the multiplicity of eigenvalues ± 1, the spectral radius, the nullity of E_n^2. Furthermore, the energy, Estrada index and the number of Kekulé structures of E_n^2 are determined.

Keywords: hexagonal system; characteristic polynomial; nullity; energy; Estrada index; Kekulé structure.

AMS Subject classification: 05C50

1 Introduction

Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $A(G)$ be the *adjacency matrix* of G. Denote by d_i the degree of the vertex v_i and $D(G) = diag(d_1, d_2, \ldots, d_n)$ the diagonal matrix. The *signless Laplacian matrix* is defined as $Q(G) = D(G) + A(G)$. The characteristic polynomial $\Phi_M(G, x) = |xI_n - M|$ is called the A and *Q-polynomial* of G if $M = A(G)$ and $Q(G)$, respectively. Since A and Q are real symmetric matrices, their eigenvalues $\lambda_1(G), \lambda_2(G), ..., \lambda_n(G)$ and $q_1(G), q_2(G), ..., q_n(G)$, respectively, are real numbers. The M-spectrum, denoted by $Spec_M(G)$, is a multiset consisting of the M-eigenvalues and $Spec_M(G)$ is called A- and Q-spectrum if $M = A(G)$ and $Q(G)$, respectively. The *nullity* of G, denoted by $\eta(G)$, is normally called the *algebraic multiplicity* of eigenvalue 0. A *Kekulé structure* K of a graph G corresponds to a *perfect matching (1-factor)* of G.

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†Corresponding author. *E-mail addresses:* huangqx@xju.edu.cn

The energy $E(G)$ of graph G, introduced by Gutman in [3], is defined as

$$E(G) = \sum_{k=1}^{n} |\lambda_k(G)|.$$

It is related to the π-electron energy in a molecule represented by a (molecular) graph. For the chemical applications and the mathematical properties of the energy of a graph, we refer to the review [4] and the recent book [5].

The Estrada index $EE(G)$ of graph G, put forward by Estrada in [6], is defined as

$$EE(G) = \sum_{k=1}^{n} e^{\lambda_k(G)}.$$

Although the Estrada index is a more newly graph-spectrum-based invariant, it has already found a remarkable variety of applications. Initially, it was used to quantify the degree of folding of long-chain molecules, especially proteins (refer to [6]). Another, fully unrelated application of Estrada index was proposed by Estrada and Rodrłguez-Vel¢zquez in [7]. They showed that Estrada index provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. Other applications of Estrada index were also reported in [8,9].

It is well-known that the theory of graph spectra is related to Chemistry through the HMO (Hückel Molecular Orbital) Theory (see [2] for an extensive review on the topic), in which there are some problems to attract many mathematicians and chemists attentions, especially the the nullity, the number of Kekulé structures and the spectrum of *hexagonal system* (benzenoid hydrocarbon). The spectrum of the linear, cyclic and Möbius cyclic chains are found in [10,11]. Zhang and Zhou give the explicit expressions of characteristic polynomials of an homologous series of benzenoid systems in [12]. Recently, Lou and Huang obtain the characteristic polynomial and spectrum of hexagonal systems H_3^n in [13]. As our knowledge, there are few of hexagonal systems whose spectra are explicitly presented except for the linear, cyclic and Möbius cyclic chains and H_3^n, and energy and Estrada index of hexagonal systems are not explicitly given so far.

In the present work, we focus on giving the characteristic polynomials and spectrum for the hexagonal system E_n^2 shown in Fig.2(a). Furthermore, the nullity, energy, Estrada index and the number of Kekulé structures of E_n^2 are also determined.

2 Elementary

In this section, we give some lemmas for the later use.

Let C_n be a cycle with n vertices. In this paper, we denote the signless Laplacian matrix of C_n by Q_n , and B_n the incidence matrix. It is clear that

$$B_nB_n^{\mathrm{T}} = \begin{pmatrix} 1 & & & & 1 \\ 1 & 1 & & & \\ & 1 & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & & & \\ & 1 & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & 1 \\ 1 & & & & 1 \end{pmatrix} = D(C_n) + A(C_n) = Q_n.$$

Lemma 2.1 ([15]). *Let C_n be the cycle on n vertices. Then the Q-polynomial of C_n is*

$$\Phi_Q(C_n, q) = \prod_{j=1}^{n}(q - 2 - 2\cos\tfrac{2\pi j}{n}).$$

It immediately follows the result from Lemma 2.1.

Corollary 2.1. *The eigenvalues of Q_n are $q_j = 2 + 2\cos\frac{2\pi j}{n}$, $j = 1, 2, \ldots, n$.*

The following result is well known.

Lemma 2.2. *Let A and B be $n \times n$ matrices. Then* $\begin{vmatrix} A & B \\ B & A \end{vmatrix} = |A + B||A - B|$.

For given bipartite graph G with the bipartite partition $V(G) = V_1 \cup V_2$ such that V_i $(i = 1, 2)$ is independent, Heibronner in [14] introduced two H-graphs of G, denoted by $H_{V_1}(G)$ and $H_{V_2}(G)$ respectively. Here we prefer to redefine $H_{V_i}(G)$ $(i = 1, 2)$ by graph terminology. $H_{V_i}(G)$ $(i = 1, 2)$ is the graph obtained from G with the vertex set V_i and two vertices $u, v \in V_i$ are joining with t edges if and only if u and v have t common neighbors in G, additionally, each vertex $u \in V_i$ is added d_u loops.

For example, we show the linear hexagonal chain L_5 with bipartite partition $V(L_5) = V_1 \cup V_2$ where V_1 is colored with black and V_2 with white, its H-graphs are isomorphic and shown in Fig.1(a) and (b), in which there is number labeled at each vertex that stands for the number of loops at it.

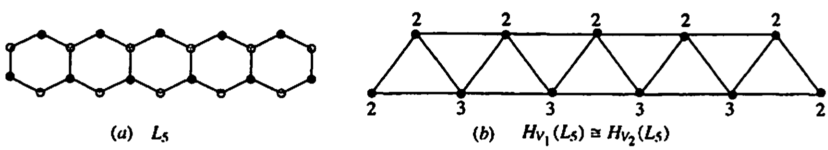

Figure 1: The linear hexagonal chain L_5 and its H-graph $H_{V_1}(L_5)$ $(H_{V_2}(L_5))$

The adjacency matrices $A(G)$ of bipartite graph G can be presented by

$$A(G) = \begin{pmatrix} 0 & B \\ B^{\mathrm{T}} & 0 \end{pmatrix} \tag{1}$$

In the following, we give the useful Lemma.

Lemma 2.3. *Let G be a bipartite graph on $n = n_1 + n_2$ vertices with bipartite partition $V(G) = V_1 \cup V_2$, and $|V_i| = n_i$ $(i = 1, 2)$. Then*

$$\Phi_A(G, x) = x^{n_2 - n_1}\Phi_A(H_1, x^2) = x^{n_1 - n_2}\Phi_A(H_2, x^2).$$

where $H_1 = H_{V_1}(G)$ and $H_2 = H_{V_2}(G)$ are the H-graphs of G.

Proof. Let $A(G)$ be the adjacency matrix of G shown in (1). By the definition of H-graphs, it is easy to see that H_1 is exactly the graph with adjacency matrix $A(H_1) = BB^T$ and H_2 with adjacency matrix $A(H_2) = B^TB$. Thus, we have

$$\Phi_A(H_1, x) = |xI_{n_1} - A(H_1)| = |xI_{n_1} - BB^T| \tag{2}$$

Additionally, in accordance with (1), we also have

$$\Phi_A(G, x) = \left|xI_n - A(G)\right| = \begin{vmatrix} xI_{n_1} & -B \\ -B^T & xI_{n_2} \end{vmatrix} = x^{n_2-n_1}|x^2I_{n_1} - BB^T| \tag{3}$$

Hence, from the (13) and (3), we immediately obtain

$$\Phi_A(G, x) = x^{n_2-n_1}\Phi_A(H_1, x^2).$$

Similarly, we have

$$\Phi_A(G, x) = x^{n_1-n_2}\Phi_A(H_2, x^2).$$

It completes this proof. □

3 The characteristic polynomial and the spectrum of E_n^2

In this section, we focus on determining the characteristic polynomial of E_n^2. Subsequently, we also give the spectral radius, the multiplicity eigenvalues ±1, the nullity and the number of Kekulé structures of E_n^2.

Let E_n^2 be the hexagonal system consisting of $3n$ ($n \geq 2$) hexagons which is shown in Fig.2(a), where two v_1's are identified as one vertex and the same as u_1's and u_2's. Since E_n^2 is bipartite graph with bipartite partition $V(E_n^2) = V_1 \cup V_2$, we color the independent set V_1 with black and V_2 with white. Clearly, $|V_1| = |V_2|$, and the two H-graphs of E_n^2 are isomorphic, i.e., $H_{V_1}(E_n^2) \cong H_{V_2}(E_n^2)$ (shorted for $H_1 \cong H_2$)), which are shown in Fig.2(b) where two w_{21}'s are identified as one vertex and the same as w_{41}'s.

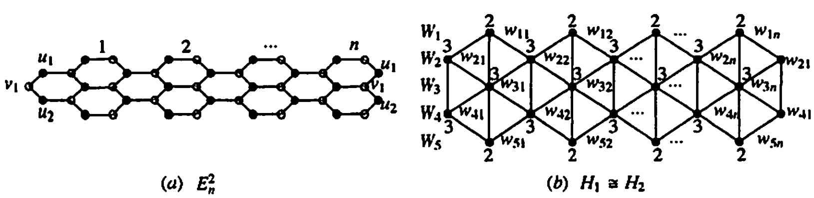

Figure 2: The plane representation of E_n^2 and its H-graphs $H_1 \cong H_2$

Now we partition the vertices of H_1 into five parts: $V(H_1) = W_1 \cup W_2 \cup \cdots \cup W_5$, where $W_i = \{w_{i1}, w_{i2}, ..., w_{in}\}$ ($i = 1, 2, ..., 5$). Clearly, $|V(H_1)| = 5n$. Let $A(H_1)$ be the adjacency matrix of H_1 and $A(W_i, W_j) = (a_{kl})_{n\times n}$ $(1 \leq i, j \leq 5)$ denote the block matrix of $A(H_1)$ corresponding W_i (the row-set) and W_j (the column-set), where $a_{kl} = 1$ if $w_{ik} \in W_i$ is adjacent with $w_{jl} \in W_j$ in H_1, and $a_{kl} = 0$ otherwise. It is easy to see that $A(W_i, W_j)^{\mathrm{T}} = A(W_j, W_i)$. For instance,

$$A(W_1, W_2) = \begin{array}{c} \\ w_{11} \\ w_{12} \\ w_{13} \\ \vdots \\ w_{1n} \end{array} \begin{array}{c} \begin{array}{ccccc} w_{21} & w_{22} & \cdots & w_{2,n-1} & w_{2n} \end{array} \\ \begin{pmatrix} 1 & 1 & & & \\ & 1 & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & 1 \\ 1 & & & & 1 \end{pmatrix}_{n\times n} \end{array} = B_n^{\mathrm{T}}.$$

Thus, according to the partition of vertices in Fig.2 (b), we have

$$\begin{cases} A(W_1, W_1) = A(W_5, W_5) = 2I_n, \\ A(W_2, W_2) = A(W_3, W_3) = A(W_4, W_4) = 3I_n, \\ A(W_1, W_2) = A(W_3, W_4) = B_n^{\mathrm{T}}, \\ A(W_2, W_3) = A(W_4, W_5) = B_n, \\ A(W_1, W_3) = A(W_2, W_4) = A(W_3, W_5) = I_n. \end{cases}$$

and the other block matrix $A(W_i, W_j)$ equals 0. Hence, we can represent the adjacency matrix of H_1 as in the form of block-matrix in terms of the ordering of $W_1, W_1, ..., W_5$ as follows:

$$A(H_1) = \begin{pmatrix} 2I_n & B_n^{\mathrm{T}} & I_n & 0 & 0 \\ B_n & 3I_n & B_n & I_n & 0 \\ I_n & B_n^{\mathrm{T}} & 3I_n & B_n^{\mathrm{T}} & I_n \\ 0 & I_n & B_n & 3I_n & B_n \\ 0 & 0 & I_n & B_n^{\mathrm{T}} & 2I_n \end{pmatrix} \tag{4}$$

In the following, we give an useful lemma to prove our main result.

Lemma 3.1. *Let H_1 be a H-graph of the hexagonal system E_n^2 that contains $3n$ $(n \geq 2)$ hexagons shown in Fig.2(a). Then the characteristic polynomial of H_1 is given by*

$$\Phi_A(H_1, x) = (x-1)^n \prod_{j=1}^{n} (x^2 - 8x + 16 - 3q_j)(x^2 - 4x + 4 - q_j)$$

where $q_j = 2 + 2\cos\frac{2\pi j}{n}$, $j = 1, 2, ..., n$.

Proof. According to (4), the characteristic polynomial of H_1 can be presented as

$$\Phi_A(H_1, x) = \det(xI_{5n} - A(H_1)) \tag{5}$$

where

$$xI_{5n} - A(H_1) = \begin{pmatrix} (x-2)I_n & -B_n^{\mathrm{T}} & -I_n & 0 & 0 \\ -B_n & (x-3)I_n & -B_n & -I_n & 0 \\ -I_n & -B_n^{\mathrm{T}} & (x-3)I_n & -B_n^{\mathrm{T}} & -I_n \\ 0 & -I_n & B_n & (x-3)I_n & -B_n \\ 0 & 0 & -I_n & -B_n^{\mathrm{T}} & (x-2)I_n \end{pmatrix}.$$

Denote by N_1 and N_2 respectively the elementary block matrices below,

$$N_1 = \begin{pmatrix} I_n & 0 & 0 & 0 & 0 \\ \frac{B_n}{x-2} & I_n & 0 & 0 & 0 \\ \frac{I_n}{x-2} & 0 & I_n & 0 & \frac{I_n}{x-2} \\ 0 & 0 & 0 & I_n & \frac{B_n}{x-2} \\ 0 & 0 & 0 & 0 & I_n \end{pmatrix}, \quad N_2 = \begin{pmatrix} I_n & 0 & 0 & 0 & 0 \\ 0 & I_n & \frac{B_n}{x-4} & 0 & 0 \\ 0 & 0 & I_n & 0 & 0 \\ 0 & 0 & \frac{B_n}{x-4} & I_n & 0 \\ 0 & 0 & 0 & 0 & I_n \end{pmatrix}.$$

First, left multiplying $xI_{5n} - A(H_1)$ by the elementary block matrix N_1, we obtain

$$N_1 \cdot (xI_{5n} - A(H_1)) = A_1 \tag{6}$$

where

$$A_1 = \begin{pmatrix} (x-2)I_n & -B_n^{\mathrm{T}} & -I_n & 0 & 0 \\ 0 & (x-3)I_n - \frac{B_nB_n^{\mathrm{T}}}{x-2} & -\frac{x-1}{x-2}B_n & -I_n & 0 \\ 0 & -\frac{x-1}{x-2}B_n^{\mathrm{T}} & \frac{(x-1)(x-4)}{x-2}I_n & -\frac{x-1}{x-2}B_n^{\mathrm{T}} & 0 \\ 0 & -I_n & -\frac{x-1}{x-2}B_n & (x-3)I_n - \frac{B_nB_n^{\mathrm{T}}}{x-2} & 0 \\ 0 & 0 & -I_n & -B_n^{\mathrm{T}} & (x-2)I_n \end{pmatrix}.$$

Similarly, left multiplying A_1 by the elementary block matrix N_2, we obtain

$$N_2 \cdot A_1 = A_2 \tag{7}$$

where

$$A_2 = \begin{pmatrix} (x-2)I_n & -B_n^{\mathrm{T}} & -I_n & 0 & 0 \\ 0 & (x-3)I_n - \frac{2x-5}{(x-2)(x-4)}B_nB_n^{\mathrm{T}} & 0 & -I_n - \frac{x-1}{(x-2)(x-4)}B_nB_n^{\mathrm{T}} & 0 \\ 0 & -\frac{x-1}{x-2}B_n^{\mathrm{T}} & \frac{(x-1)(x-4)}{x-2}I_n & -\frac{x-1}{x-2}B_n^{\mathrm{T}} & 0 \\ 0 & -I_n - \frac{x-1}{(x-2)(x-4)}B_nB_n^{\mathrm{T}} & 0 & (x-3)I_n - \frac{2x-5}{(x-2)(x-4)}B_nB_n^{\mathrm{T}} & 0 \\ 0 & 0 & -I_n & -B_n^{\mathrm{T}} & (x-2)I_n \end{pmatrix}.$$

Recall that $B_nB_n^{\mathrm{T}} = Q_n$, the signless Laplacian matrix of C_n. Now we expand the determinant of A_2 according to its 1th-, 5th- and 3th-columns and get

$$\det(A_2) = (x-2)^n(x-1)^n(x-4)^n \det(A_3) \tag{8}$$

where

$$A_3 = \begin{pmatrix} (x-3)I_n - \frac{2x-5}{(x-2)(x-4)}Q_n & -I_n - \frac{x-1}{(x-2)(x-4)}Q_n \\ -I_n - \frac{x-1}{(x-2)(x-4)}Q_n & (x-3)I_n - \frac{2x-5}{(x-2)(x-4)}Q_n \end{pmatrix}.$$

By Lemma 2.2, we have

$$\begin{aligned} \det(A_3) &= \begin{vmatrix} (x-3)I_n - \frac{2x-5}{(x-2)(x-4)}Q_n & -I_n - \frac{x-1}{(x-2)(x-4)}Q_n \\ -I_n - \frac{x-1}{(x-2)(x-4)}Q_n & (x-3)I_n - \frac{2x-5}{(x-2)(x-4)}Q_n \end{vmatrix} \\ &= \left|(x-3)I_n - \frac{2x-5}{(x-2)(x-4)}Q_n - I_n - \frac{x-1}{(x-2)(x-4)}Q_n\right| \times \left|(x-3)I_n - \frac{2x-5}{(x-2)(x-4)}Q_n + I_n + \frac{x-1}{(x-2)(x-4)}Q_n\right| \\ &= \left|-\frac{3}{x-4}Q_n + (x-4)I_n\right| \times \left|-\frac{1}{x-2}Q_n + (x-2)I_n\right|. \end{aligned}$$

Note that $\det(N_1) = 1$ and $\det(N_2) = 1$. From Eqs. (5)-(8), we have

$$\begin{aligned}\Phi_A(H_1, x) &= \det(A_2) = (x-2)^n(x-1)^n(x-4)^n \det(A_3) \\ &= (x-2)^n(x-1)^n(x-4)^n \left| -\tfrac{3}{x-4}Q_n + (x-4)I_n \right| \times \left| -\tfrac{1}{x-2}Q_n + (x-2)I_n \right| \\ &= (x-1)^n \left| (x^2-8x+16)I_n - 3Q_n \right| \times \left| (x^2-4x+4)I_n - Q_n \right|\end{aligned} \tag{9}$$

From Corollary 2.1, we know that $q_j = 2 + 2\cos\frac{2\pi j}{n}$ are the eigenvalues of Q_n. Finally, from Eq.(9) we have

$$\Phi_A(H_1, x) = (x-1)^n \prod_{j=1}^{n} (x^2 - 8x + 16 - 3q_j)(x^2 - 4x + 4 - q_j) \ .$$

It completes this proof. □

In the following, according to the Lemma 3.1, we give our main result.

Theorem 3.1. *Let E_n^2 be the hexagonal system with $3n$ ($n \geq 2$) hexagons shown in Fig.2(a). Then the characteristic polynomial of E_n^2 is represented by*

$$\Phi_A(E_n^2, x) = (x^2-1)^n \prod_{j=1}^{n} (x^4 - 8x^2 + 16 - 3q_j)(x^4 - 4x^2 + 4 - q_j) \tag{10}$$

where $q_j = 2 + 2\cos\frac{2\pi j}{n}$ is the Q-eigenvalue of C_n.

Proof. Note that the bipartite graph E_n^2 has vertex partition $V = V_1 \cup V_2$ such that $|V_1| = |V_2|$, where the vertices of V_1 are colored with black and of V_2 with white (see in Fig.2(a)), and H_1 is its H-graph (see in Fig.2(b)). By Lemma 2.3 and Lemma 3.1, we obtain

$$\begin{aligned}\Phi_A(E_n^2, x) &= \Phi_A(H_1, x^2) \\ &= (x^2-1)^n \prod_{j=1}^{n} (x^4 - 8x^2 + 16 - 3q_j)(x^4 - 4x^2 + 4 - q_j).\end{aligned}$$

It completes this proof. □

As an application of Theorem 3.1, we give an example to find the characteristic polynomial and spectrum of E_n^2.

Example 1. *For $n = 3$, E_n^2 has 9 hexagons and 30 vertices. By Theorem 3.1, $q_1 = 1$, $q_2 = 1$ and $q_3 = 4$, and thus*

$$\begin{aligned}&f_1(x) = x^4 - 8x^2 + 13, \quad f_2(x) = x^4 - 8x^2 + 13, \quad f_3(x) = x^4 - 8x^2 + 4; \\ &g_1(x) = x^4 - 4x^2 + 3, \quad g_2(x) = x^4 - 4x^2 + 3, \quad g_3(x) = x^4 - 4x^2.\end{aligned}$$

By simple calculation, we obtain the characteristic polynomial of E_n^2 from Eq.(10):

$$\begin{aligned}\Phi_A(E_3^2, x) &= (x^2-1)^3 \prod_{j=1}^{3} f_j(x) g_j(x) \\ &= x^{30} - 39x^{28} + 675x^{26} - 6865x^{24} + 45798x^{22} - 211878x^{20} + 700746x^{18} \\ &\quad -1682910x^{16} + 2949777x^{14} - 3757279x^{12} + 3426627x^{10} - 2172177x^8 \\ &\quad +905800x^6 - 222612x^4 + 24336x^2.\end{aligned}$$

The spectrum of E_3^2 is given in Table 1.

Table 1 The spectrum of E_3^2

polynomial	*eigenvalues*					
$f_1(x)$	2.3942	1.5060	−2.3942	−1.5060		
$f_2(x)$	2.3942	1.5060	−2.3942	−1.5060		
$f_3(x)$	2.7321	0.7321	−2.7321	−0.7321		
$g_1(x)$	1.7321	1	−1.7321	−1		
$g_2(x)$	1.7321	1	−1.7321	−1		
$g_3(x)$	0	0	2	−2		
$(x^2-1)^3$	−1	−1	−1	1	1	1

Lemma 3.2. *Let* $f(x) = \prod_{j=1}^{n}(x^4 - 8x^2 + 16 - 3q_j)$ *where* $q_j = 2 + 2\cos\frac{2\pi j}{n}$ *are the* Q*-eigenvalue of* C_n*. Then we have*

(1) $\lambda_{1j}^{+} = \sqrt{4+\sqrt{3q_j}}$, $\lambda_{1j}^{-} = -\sqrt{4+\sqrt{3q_j}}$, $\lambda_{2j}^{+} = \sqrt{4-\sqrt{3q_j}}$ *and* $\lambda_{2j}^{-} = -\sqrt{4-\sqrt{3q_j}}$ *are roots of* $f(x)$ *where* $j = 1, 2, ..., n$.

(2) each root of $f(x)$ *has multiplicity* 2 *except for the simple roots* $\pm\sqrt{4+2\sqrt{3}}$ *and* $\pm\sqrt{4-2\sqrt{3}}$.

Proof. Let $f_j(x) = x^4 - 8x^2 + 16 - 3q_j$. Then $f(x) = \prod_{j=1}^{n} f_j(x)$. Note that

$$\begin{aligned} f_j(x) &= (x^2 - (4+\sqrt{3q_j}))(x^2 - (4-\sqrt{3q_j})) \\ &= (x-\sqrt{4+\sqrt{3q_j}})(x+\sqrt{4+\sqrt{3q_j}})(x-\sqrt{4-\sqrt{3q_j}})(x+\sqrt{4-\sqrt{3q_j}}) \end{aligned}$$

It follows (1).

(2) Clearly, $\lambda_{1j}^{+} > \lambda_{1j}^{-}$, $\lambda_{1j}^{+} > \lambda_{2j}^{-}$ and $\lambda_{1j}^{+} = \lambda_{2j}^{+}$ if and only if $\lambda_{1,\frac{n}{2}}^{+} = 2 = \lambda_{2,\frac{n}{2}}^{+}$. $\lambda_{1j}^{-} < \lambda_{1j}^{+}$, $\lambda_{1j}^{-} < \lambda_{2j}^{+}$ and $\lambda_{1j}^{-} = \lambda_{2j}^{-}$ if and only if $\lambda_{1,\frac{n}{2}}^{-} = -2 = \lambda_{2,\frac{n}{2}}^{-}$. It now leaves to distinguish $\{\lambda_{1j}^{+} \mid j = 1, 2, ..., n\}$, $\{\lambda_{1j}^{-} \mid j = 1, 2, ..., n\}$, $\{\lambda_{2j}^{+} \mid j = 1, 2, ..., n\}$ and $\{\lambda_{2j}^{-} \mid j = 1, 2, ..., n\}$ themselves.

Suppose that n is even. By simply observation, we know that $\lambda_{1j}^{+} = \lambda_{1,n-j}^{+}$, $\lambda_{1j}^{-} = \lambda_{1,n-j}^{-}$, $\lambda_{2j}^{+} = \lambda_{2,n-j}^{+}$, $\lambda_{2j}^{-} = \lambda_{2,n-j}^{-}$ where $j = 1, 2, ..., \frac{n}{2} - 1$. These are all roots of multiplicity 2. In addition, $\lambda_{1,\frac{n}{2}}^{+} = 2 = \lambda_{2,\frac{n}{2}}^{+}$, $\lambda_{1,\frac{n}{2}}^{-} = -2 = \lambda_{2,\frac{n}{2}}^{-}$ are also two roots of multiplicity 2. Whereas $\lambda_{1n}^{+} = \sqrt{4+2\sqrt{3}}$, $\lambda_{1n}^{-} = -\sqrt{4+2\sqrt{3}}$, $\lambda_{2n}^{+} = \sqrt{4-2\sqrt{3}}$ and $\lambda_{2n}^{-} = -\sqrt{4-2\sqrt{3}}$ are four simple roots.

Suppose that n is odd. Similarly, $\lambda_{1j}^{+} = \lambda_{1,n-j}^{+}$, $\lambda_{1j}^{-} = \lambda_{1,n-j}^{-}$, $\lambda_{2j}^{+} = \lambda_{2,n-j}^{+}$, $\lambda_{2j}^{-} = \lambda_{2,n-j}^{-}$ where $j = 1, 2, ..., \frac{n-1}{2}$ are all roots of multiplicity 2. Whereas $\lambda_{1n}^{+} = \sqrt{4+2\sqrt{3}}$, $\lambda_{1n}^{-} = -\sqrt{4+2\sqrt{3}}$, $\lambda_{2n}^{+} = \sqrt{4-2\sqrt{3}}$ and $\lambda_{2n}^{-} = -\sqrt{4-2\sqrt{3}}$ are four simple roots.

It follows our result. □

By the same method as in the proof of Lemma 3.2, one can verify our following result.

Lemma 3.3. *Let* $g(x) = \prod_{j=1}^{n}(x^4 - 4x^2 + 4 - q_j)$ *where* $q_j = 2 + 2\cos\frac{2\pi j}{n}$ *are the Q-eigenvalue of* C_n. *Then we have*

(1) $\lambda_{3j}^+ = \sqrt{2+\sqrt{q_j}}$, $\lambda_{3j}^- = -\sqrt{2+\sqrt{q_j}}$, $\lambda_{4j}^+ = \sqrt{2-\sqrt{q_j}}$ *and* $\lambda_{4j}^- = -\sqrt{2-\sqrt{q_j}}$ *are roots of* $g(x)$ *where* $j = 1, 2, ..., n$.

(2) each root of $g(x)$ *has multiplicity 2 except for the simple roots* ± 2.

Taking the symbols in Lemma 3.2 and 3.3, the formula of Theorem 3.1 can be represented by

$$\begin{aligned}\Phi_A(E_n^2, x) &= (x^2-1)^n \prod_{j=1}^{n}(x^4 - 8x^2 + 16 - 3q_j)(x^4 - 4x^2 + 4 - q_j)\\ &= (x^2-1)^n f(x) g(x).\end{aligned}$$

Summarizing Lemma 3.2 and 3.3, we can roughly determine the multiplicity of eigenvalues of E_n^2.

Theorem 3.2. *Let* E_n^2 *be the hexagonal system with* $3n$ $(n \geq 2)$ *hexagons shown in Fig.2(a), and let* $q_j = 2 + 2\cos\frac{2\pi j}{n}$ *be the Q-eigenvalue of* C_n. *Then we have*

(1) $Spec_A(E_n^2) = A \cup B \cup C$, *where* $A = \{\lambda_{ij}^+, \lambda_{ij}^- \mid i = 1, 2; j = 1, 2, ..., n\}$ *and* $\lambda_{1j}^+, \lambda_{2j}^+, \lambda_{1j}^-, \lambda_{2j}^-$ *are defined in Lemma 3.2;* $B = \{\lambda_{ij}^+, \lambda_{ij}^- \mid i = 3, 4; j = 1, 2, ..., n\}$ *and* $\lambda_{3j}^+, \lambda_{4j}^+, \lambda_{3j}^-, \lambda_{4j}^-$ *are defined in Lemma 3.3;* $C = \{1^n, -1^n\}$.

(2) each eigenvalue in A has multiplicity 2 except for the simple roots $\pm\sqrt{4+2\sqrt{3}}$ *and* $\pm\sqrt{4-2\sqrt{3}}$.

(3) each eigenvalue in B has multiplicity 2 except for the simple roots ± 2.

It is worth to mention that the joint of A and B is not necessarily empty (it seems difficult to determine $A \cap B$). For instance, we can verify that $\pm 1 \in A \cap B$. In fact, $\pm 1 = \lambda_{2,\frac{n}{6}}^{\pm}$ and $\pm 1 = \lambda_{4,\frac{n}{3}}^{\pm}$ (see Corollary 3.2).

Corollary 3.1. *For any positive integers* $n \geq 2$, E_n^2 *has spectral radius* $\rho(E_n^2) = \sqrt{4+2\sqrt{3}}$.

Proof. By the Theorem 3.2, we know that $Spec_A(E_n^2) = \{\lambda_{ij}^+, \lambda_{ij}^- \mid i = 1, 2, 3, 4; j = 1, 2, ..., n\}$. It is easy to see that the largest eigenvalues of E_n^2 lies in $\{\lambda_{1j}^+ = \sqrt{4+\sqrt{3q_j}} \mid j = 1, 2, ..., n\}$. Since $q_j = 2 + 2\cos\frac{2\pi j}{n}$ $(1 \leq j \leq n)$, $q_n = 4$ and $q_j < 4$ if $j = 1, 2, ..., n-1$. Hence, $\rho(E_n^2) = \sqrt{4+2\sqrt{3}}$. □

Denote by $m(\lambda)$ the multiplicity of eigenvalue λ of G. Although $A \cap B$ can not be exactly determined, we can determine $m(1)$ and $m(-1)$ for $\pm 1 \in A \cap B$.

Corollary 3.2. *Let E_n^2 be hexagonal system with $3n$ ($n \geq 2$) hexagons. Then $m(1) = m(-1)$, and*

$$m(1) = \begin{cases} n+4 & \text{if } n \equiv 0 (\text{mod} 6), \\ n+2 & \text{if } n \equiv 3 (\text{mod} 6), \\ n & \text{Otherwise.} \end{cases}$$

Proof. From the Theorem 3.2, we know that $m(1) \geq n$ and $m(-1) \geq n$. In addition, $\lambda_{1j}^+ \geq 2$, $\lambda_{1j}^- \leq -2$, $\lambda_{3j}^+ \geq \sqrt{2}$ and $\lambda_{3j}^- \leq -\sqrt{2}$. Thus, we need only to consider if $\lambda_{ij}^+ = 1$ and $\lambda_{ij}^- = -1$ for some $i \in \{2, 4\}$ and $j \in \{1, 2, ..., n\}$.

It is clear that $\lambda_{2j}^+ = 1$ (or $\lambda_{2j}^- = -1$) if and only if $3 - q_j = 0$ (that is, $q_j = 2 + 2\cos\frac{2\pi j}{n} = 3$) if and only if $j = \frac{n}{6} \in \{1, 2, \ldots, n\}$. Similarly, $\lambda_{4j}^+ = 1$ (or $\lambda_{4j}^- = -1$) if and only if $1 - q_j = 0$ (that is, $q_j = 2 + 2\cos\frac{2\pi j}{n} = 1$) if and only if $j = \frac{n}{3} \in \{1, 2, \ldots, n\}$. By the above arguments and Theorem 3.2, if $n \equiv 0(\text{mod}6)$ then $\lambda_{2,\frac{n}{6}}^+ = \lambda_{4,\frac{n}{3}}^+ = 1$ contribute 4 to $m(1)$; if $n \equiv 3(\text{mod}6)$ then $\lambda_{4,\frac{n}{3}}^+ = 1$ contribute 2 to $m(1)$, otherwise contribute 0.

It is the same if we consider $m(-1)$. The result follows. □

The following result gives the nullity of E_n^2.

Corollary 3.3. $\eta(E_n^2) = 2$.

Proof. We see from Theorem 3.2 that $\lambda_{ij}^+ \neq 0$ and $\lambda_{ij}^- \neq 0$ except for $\lambda_{4n}^+ = \lambda_{4n}^- = 0$. It follows $\eta(E_n^2) = 2$. □

4 The energy and the Estrada index of E_n^2

In this section, we determine the energy and the Estrada index of E_n^2, respectively. By Theorem 3.2, we can obtain the accurate value and the estimated value of energy of E_n^2.

Theorem 4.1. *Let $E(E_n^2)$ be the energy of E_n^2. Then*

$$E(E_n^2) = 2n + 2\sum_{j=1}^{n}\left(\sqrt{4 + 2\sqrt{3}\cos\frac{\pi j}{n}} + \sqrt{4 - 2\sqrt{3}\cos\frac{\pi j}{n}} + 2\cos\frac{\pi j}{2n} + 2\sin\frac{\pi j}{2n}\right) \quad (11)$$

Proof. Note that $\sqrt{q_j} = \sqrt{2 + 2\cos\frac{2\pi j}{n}} = 2|\cos\frac{\pi j}{n}|$ where $j = 1, 2, ..., n$. We have $\sqrt{q_j} = 2\cos\frac{\pi j}{n}$ if $j \in \{1, 2, ..., \lfloor\frac{n-1}{2}\rfloor\}$; $\sqrt{q_j} = -2\cos\frac{\pi j}{n}$ if $j \in \{\lfloor\frac{n-1}{2}\rfloor + 1, \lfloor\frac{n-1}{2}\rfloor + 2, ..., n\}$. Hence, by Theorem 3.2, we have

$$\lambda_{1j}^+ = \sqrt{4 + 2\sqrt{3}\cos\frac{\pi j}{n}},\ \lambda_{2j}^+ = \sqrt{4 - 2\sqrt{3}\cos\frac{\pi j}{n}},\ \lambda_{3j}^+ = 2\cos\frac{\pi j}{2n},\ \lambda_{4j}^+ = 2\sin\frac{\pi j}{2n}$$

where $j \in \{1, 2, \ldots, \lfloor \frac{n-1}{2} \rfloor\}$, and

$$\lambda^+_{1j} = \sqrt{4 - 2\sqrt{3}\cos\frac{\pi j}{n}},\ \lambda^+_{2j} = \sqrt{4 + 2\sqrt{3}\cos\frac{\pi j}{n}},\ \lambda^+_{3j} = 2\sin\frac{\pi j}{2n},\ \lambda^+_{4j} = 2\cos\frac{\pi j}{2n}$$

where $j \in \{\lfloor \frac{n-1}{2} \rfloor + 1, \lfloor \frac{n-1}{2} \rfloor + 2, \ldots, n\}$. Thus, we immediately obtain

$$\begin{aligned} E(E_n^2) &= \sum_{j=1}^{10n} |\lambda_j(E_n^2)| \\ &= 2n + 2\sum_{j=1}^{n}\left(\sqrt{4+2\sqrt{3}\cos\frac{\pi j}{n}} + \sqrt{4-2\sqrt{3}\cos\frac{\pi j}{n}} + 2\cos\frac{\pi j}{2n} + 2\sin\frac{\pi j}{2n}\right). \end{aligned}$$

It follows our result. □

Corollary 4.1. *Let $E(E_n^2)$ be the energy of E_n^2. Then*

$$\lim_{n\to\infty} \frac{E(E_n^2)}{n} = 2 + \frac{4}{\pi}\int_0^\pi \sqrt{4 + 2\sqrt{3}\cos x}\,dx + \frac{16}{\pi} \approx 14.6117.$$

Proof. By the definition of definite integral, we have

$$\lim_{n\to\infty} \frac{1}{n}\sum_{j=1}^{n} \sqrt{4+2\sqrt{3}\cos\frac{\pi j}{n}} = \int_0^1 \sqrt{4+2\sqrt{3}\cos \pi t}\,dt = \frac{1}{\pi}\int_0^\pi \sqrt{4+2\sqrt{3}\cos x}\,dx,$$

$$\lim_{n\to\infty} \frac{1}{n}\sum_{j=1}^{n} 2\cos\frac{\pi j}{2n} = \int_0^1 2\cos\frac{\pi t}{2}\,dt = \frac{1}{\pi}\int_0^\pi 2\cos\frac{\theta}{2}\,d\theta = \frac{4}{\pi}\int_0^{\frac{\pi}{2}} \cos x\,dx = \frac{4}{\pi}.$$

In addition, note that $\cos\frac{\pi j}{n} = -\cos\frac{(n-j)\pi}{n}$, we have

$$\lim_{n\to\infty} \frac{1}{n}\sum_{j=1}^{n} \sqrt{4-2\sqrt{3}\cos\frac{\pi j}{n}} = \lim_{n\to\infty} \frac{1}{n}\sum_{j=1}^{n} \sqrt{4+2\sqrt{3}\cos\frac{(n-j)\pi}{n}} = \frac{1}{\pi}\int_0^\pi \sqrt{4+2\sqrt{3}\cos x}\,dx,$$

$$\lim_{n\to\infty} \frac{1}{n}\sum_{j=1}^{n} 2\sin\frac{\pi j}{2n} = \int_0^1 2\sin\frac{\pi t}{2}\,dt = \int_0^1 2\cos\left(\frac{\pi}{2} - \frac{\pi t}{2}\right)dt = \frac{4}{\pi}\int_0^{\frac{\pi}{2}} \cos x\,dx = \frac{4}{\pi}.$$

Since the original function of $l(x) = \sqrt{4 + 2\sqrt{3}\cos x}$ was not be found, with the help of Matlab, we easily compute the approximate value: $\int_0^\pi \sqrt{4 + 2\sqrt{3}\cos x}\,dx \approx 5.9052$.

It follows our result by the above arguments and Theorem 4.1. □

The formula (11) is the accurate value of energy of E_n^2. By Corollary 4.1, we know that $E'(E_n^2)$=14.6117n is the estimated value of energy of E_n^2. We compare the accurate value and the estimated value of $E(E_n^2)$ from $n = 2$ to $n = 8$ in Table 2. It shows that they are very closer.

Table 2 The $E(E_n^2)$ and $E'(E_n^2)$ of E_n^2 from $n = 2$ to $n = 8$

E_n^2	E_2^2	E_3^2	E_4^2	E_5^2	E_6^2	E_7^2	E_8^2
$E(E_n^2)$	28.5851	43.4570	58.1767	72.8465	87.4948	102.1320	116.7625
$E'(E_n^2)$	29.2234	43.8351	58.4468	73.0585	87.6702	102.2819	116.8936

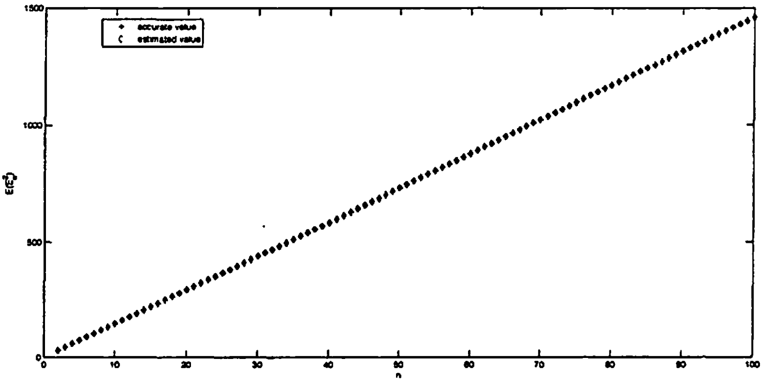

Figure 3: The accurate value $E(E_n^2)$ and the estimated value $E'(E_n^2)$ of energy of E_n^2

We further give a mathematical experiment with the help of Matlab to compare the accurate value and the estimated value in Fig.3, it indicates that they are more closer as n is larger.

By the same method of Theorem 4.1 and Corollary 4.1, from Theorem 3.2 we can obtain the following Theorem 4.2 and Corollary 4.2.

Theorem 4.2. *Let $EE(E_n^2)$ be the Estrada index of E_n^2. Then*

$$EE(E_n^2) = n(e+\tfrac{1}{e})+\sum_{j=1}^{n}\Big(e^{\sqrt{4+2\sqrt{3}\cos\frac{\pi j}{n}}}+e^{-\sqrt{4+2\sqrt{3}\cos\frac{\pi j}{n}}}+e^{\sqrt{4-2\sqrt{3}\cos\frac{\pi j}{n}}} \\ +e^{-\sqrt{4-2\sqrt{3}\cos\frac{\pi j}{n}}}+e^{2\cos\frac{\pi j}{2n}}+e^{-2\cos\frac{\pi j}{2n}}+e^{2\sin\frac{\pi j}{2n}}+e^{-2\sin\frac{\pi j}{2n}}\Big) \tag{12}$$

Corollary 4.2. *Let $EE(E_n^2)$ be the Estrada index of E_n^2. Then*

$$\lim_{n\to\infty}\frac{EE(E_n^2)}{n} = \frac{2}{\pi}\int_0^{\pi} e^{\sqrt{4+2\sqrt{3}\cos x}}+e^{-\sqrt{4+2\sqrt{3}\cos x}}\,dx+\frac{4}{\pi}\int_0^{\frac{\pi}{2}} e^{2\cos x}+e^{-2\cos x}\,dx+e+\frac{1}{e}\approx 28.7215.$$

The formula (12) is the accurate value of Estrada index of E_n^2. By Corollary 4.2, we know that $EE'(E_n^2)$=28.7215n is the estimated value of Estrada index of E_n^2. We compare the accurate value and estimated value of $EE(E_n^2)$ from n = 2 to n = 8 in Table 3. It shows that they are very closer.

Table 3 The $EE(E_n^2)$ and $EE'(E_n^2)$ of E_n^2 from n = 2 to n = 8

E_n^2	E_2^2	E_3^2	E_4^2	E_5^2	E_6^2	E_7^2	E_8^2
$EE(E_n^2)$	57.4479	86.1646	114.8861	143.6076	172.3292	201.0507	229.7722
$EE'(E_n^2)$	57.4430	86.1645	114.8860	143.6075	172.3290	201.0505	229.7720

We further give a mathematical experiment with the help of Matlab to compare the accurate value and the estimated value in Fig.4, it indicates that they are more closer as n is larger.

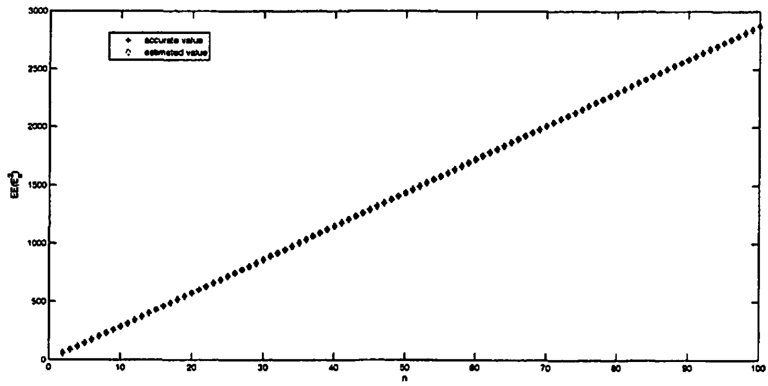

Figure 4: The accurate value $EE(E_n^2)$ and the estimated value $EE'(E_n^2)$ of Estrada index of E_n^2

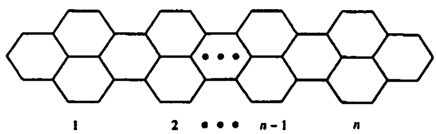

Figure 5: Hexagonal system D_n

5 The number of Kekulé structures of E_n^2

In this section, we determine the number of Kekulé structures (or perfect matchings) of E_n^2.

Denote by $K(G)$ the number of perfect matchings of G. The following formula is well known:

$$K(G) = K(G - u - v) + K(G - e) \tag{13}$$

where $e = uv$ is an edge of G. The following Fig.7 indicates the applications of formula (13) for some defined graphs that will be used in the proof of theorem 5.1.

Lemma 5.1 ([12]). *The number of perfect matchings of D_n $(n \geq 0)$ is $2 \cdot 3^n$, where hexagonal system D_n is shown in Fig. 5.*

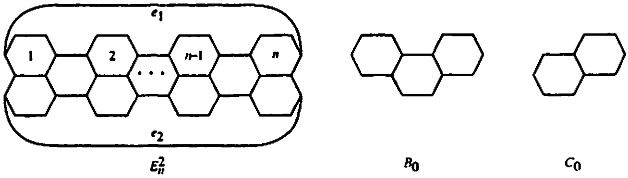

Figure 6: Hexagonal system E_n^2

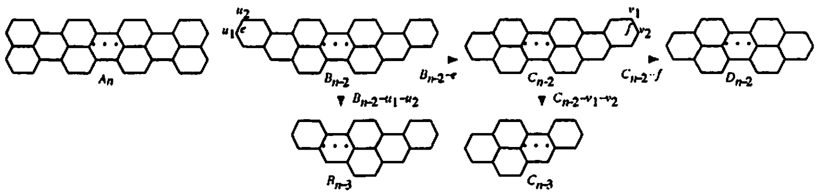

Figure 7: Enumerating the perfect matchings of E_n^2

Now we consider to enumerate the perfect matchings of E_n^2 (see Fig.6).

Theorem 5.1. *The number of perfect matchings of* E_n^2 $(n \geq 2)$ *is* $2 \cdot 3^n + 2$.

Proof. Let $M(e_1, e_2)$ be the set of the perfect matchings of E_n^2 containing e_1 and e_2, $M(\bar{e_1}, \bar{e_2})$ the set containing neither e_1 nor e_2, $M(\bar{e_1}, e_2)$ the set containing e_2 but e_1 and $M(e_1, \bar{e_2})$ the set containing e_1 but e_2. Clearly, $M(e_1, e_2) \cup M(\bar{e_1}, \bar{e_2}) \cup M(\bar{e_1}, e_2) \cup M(e_1, \bar{e_2})$ is a partition of the perfect matchings of E_n^2. For $n \geq 3$, we consider the following situations.

It is easy to see that $M(e_1, e_2)$ contains exactly one perfect matching of E_n^2.

$M \in M(\bar{e_1}, \bar{e_2})$ if and only if M is a perfect matching of A_n shown in Fig.7, and easily see that $K(A_n) = 3^n$. Hence $|M(\bar{e_1}, \bar{e_2})| = 3^n$.

We see that there exists a one-to-one correspondence between $M(\bar{e_1}, e_2)$ and the set of perfect matchings of B_{n-2} shown in Fig.7. Thus $|M(\bar{e_1}, e_2)| = K(B_{n-2})$. Let C_{n-2} be shown in Fig.7. By applying formula (13) to B_{n-2} at the edge e, we have

$$K(B_{n-2}) = K(B_{n-2} - u_1 - u_2) + K(B_{n-2} - e) = K(B_{n-3}) + K(C_{n-2}) \qquad (14)$$

Let D_{n-2} be shown in Fig.7. By applying formula (13) to C_{n-2} at the edge f, we similarly have $K(C_{n-2}) = K(C_{n-3}) + K(D_{n-2})$. By Lemma 5.1,

$$K(C_{n-2}) = K(C_{n-3}) + 2 \cdot 3^{n-2} \qquad (15)$$

Note that $c_0 = K(C_0) = 3$. By recursion (15), we obtain

$$K(C_{n-2}) = 2 \cdot 3^{n-2} + 2 \cdot 3^{n-3} + \cdots + 2 \cdot 3 + c_0 = 3^{n-1},$$

which returns to (14), we have $K(B_{n-2}) = K(B_{n-3}) + 3^{n-1}$. Note that $b_0 = K(B_0) = 5$, we recursively obtain

$$M(\bar{e}_1, e_2) = K(B_{n-2}) = 3^{n-1} + 3^{n-2} + \cdots + 3 + b_0 = \frac{3^n + 1}{2}.$$

By the symmetry of E_n^2, we know that $M(e_1, \bar{e}_2) = \frac{3^n+1}{2}$.

Finally we obtain

$$K(E_n^2) = 3^n + 1 + 2 \cdot \frac{3^n + 1}{2} = 2 \cdot 3^n + 2.$$

For $n = 2$, one can directly verify that $K(E_2^2) = 2 \cdot 3^2 + 2$. It follows our result. □

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