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Relationship between Coefficients of Characteristic Polynomial and Matching Polynomial of Regular Graphs and its Applications

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ABSTRACT

Suppose G is a graph, $A(G)$ its adjacency matrix and $\psi(G,\lambda) = \lambda^n + a_1\lambda_{n-1} + \dots + a_n$ is the characteristic polynomial of G. The matching polynomial of G is defined as $M(G,x) = m(G,0)x^n - m(G,1)x^{n-2} - m(G,2)x^{n-4} + \dots$, where $m(G,k)$ is the number of k−matchings in G. In this paper, the relationship between $2k$-th coefficient of the characteristic polynomial, a_{2k}, and k-th coefficient of the matching polynomial, $(-1)^k m(G, k)$, $k=0,1,2,\dots$, in a regular graph is determined. In addition, these relations for finding 5,6-matchings of fullerene graphs are applied.

1. INTRODUCTION

Suppose G is a simple graph with n vertices and m edges, and $A(G)$ is the adjacency matrix of G. The characteristic polynomial of G, denoted by $\psi(G,\lambda)$, is defined as:

$$\psi(G,\lambda) = \det(\lambda I_n - A(G)) = \lambda^n + a_1\lambda^{n-1} + \dots + a_{n-1}\lambda + a_n .$$

The roots of the characteristic polynomial are the eigenvalues of G. A k–matching in G is a set of k edges without common vertices. Denote the number of k–matchings in G by m(G,k). It is clear that $m(G, 1)=m$ and $m(G, k)=0$ for $k > \lfloor n/2 \rfloor$ or $k < 0$. The matching polynomial of the graph G is defined as:

$$M(G,x) = \sum_{k\geq 0} (-1)^k m(G,k) x^{n-2k} .$$

Go to [9] for details. The girth of G is the length of the shortest cycle contained in G. An edge incident to a vertex of degree one is called a pendant edge.

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Fullerenes are polyhedral cage molecules composed entirely of carbon atoms. The molecular graph of such a molecule is 3–connected and planar with faces all pentagons and hexagons. Suppose p and h are the number of pentagons and hexagons in an n–vertex fullerene F, respectively. Therefore the Euler's theorem implies that $p = 12$ and $h = n/2 - 10$. After the outstanding work of Kroto et al. [14] in discovering the buckminsterfullerene C_{60}, a lot of researchers devoted their time to find mathematical properties of these new materials. The most important book on this topic is the well known book of Fowler and Manolopoulos [12]. There are several different computer programs for working with fullerenes, one of them is developed by Myrvold and her colleagues [16]. Another program is developed by Schwerdtfeger et al. [17].

Fullerenes are also called (5, 6)–fullerenes. An ***IPR*** (5, 6)–fullerene is one for which no two pentagons share an edge. The minimum distance of two vertices of any two nearest pentagons is called the **pentadistance** of fullerene. In this paper, all (5,6)–fullerenes considered are at distance of at least 2. For more information on the fullerenes and additional results you can see [1, 4, 10, 11].

In this section, some operational definitions used in this paper are presented. The symbols P_n and C_n, stand for the path with n vertices and the cycle of size n, respectively, and $\varphi_G(H)$ or $\varphi(H)$ for the number of H–subgraphs of G. Any undefined terminology and notation can be found in [7].

Behmaram in his thesis [2] and in a recent paper [3] extended the notion of fullerene to m–generalized fullerene. By his definition, a 3–connected cubic planar graph G is called m–generalized fullerene if its faces are two m–gons and all other pentagons and hexagons. The concepts of m–generalized (3, 6)–fullerene and m–generalized (4, 6)–fullerene can be defined in a similar way [15]. We refer to Deza and his co–authors for some other generalization of fullerenes [8, 18, 19].

It is easy to see that a (3, 5, 6)–fullerene molecule with n atoms and exactly 2 triangles has 6 pentagons and $n/2-6$ hexagons. A (4, 5, 6)–fullerene molecule with n atoms and exactly 2 squares has 8 pentagons and $n/2-8$ hexagons, see Figure 1. Also a (5, 6, 7)–fullerene molecule with n atoms has exactly 14 pentagons, 2 heptagons and $n/2-14$ hexagons, and a (4, 6, 8)–fullerene molecule with n atoms has exactly 12 squares, 6 octagons and $n/2-16$ hexagons, see Figure 2. The aim of this paper is determination the relationship between $2k$–th coefficient of characteristic polynomial and k–th coefficient of matching polynomial of a regular graph with girth 5. Also in this paper we determine some coefficients of characteristic polynomial of some fullerene graphs. These coefficients are studied in [6].

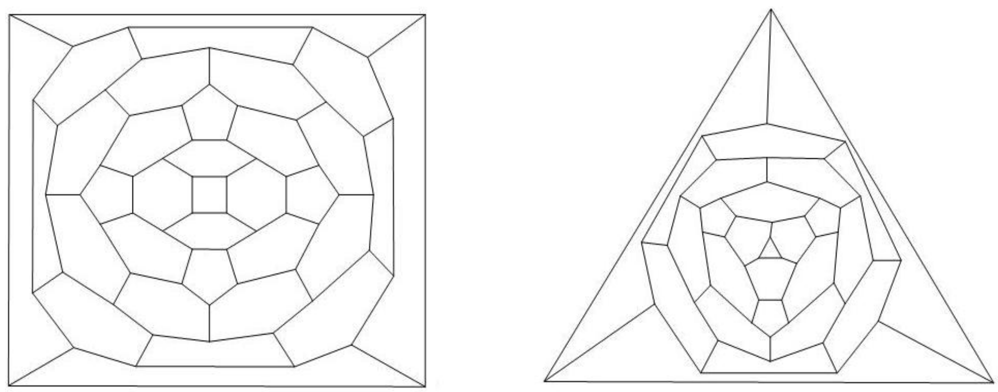


Figure 1. A (4, 5, 6)– (left) and (3, 5, 6)–Fullerene (right).

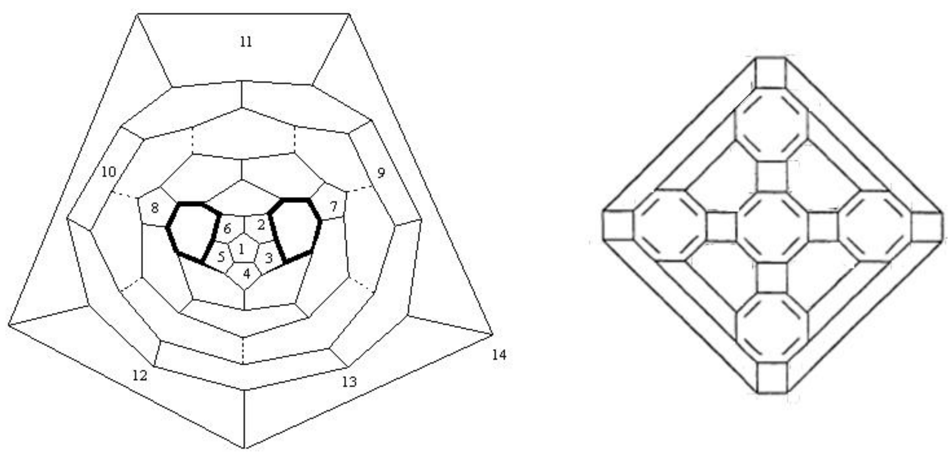


Figure 2. A (5, 6, 7)– (left) and (4, 6, 8)–Fullerene (right).

2. PRELIMINARIES

In this section, we present the definitions and the theorems that are used in the study. Suppose G is a graph with n vertices, m edges and with adjacency matrix $A(G)$. It is easy to see that if G is a regular graph of degree r, then $m=nr/2$. The characteristic polynomial of G, $\psi(G,\lambda)$, is defined as:

$$\psi(G,\lambda) = \lambda^n + a_1\lambda^{n-1} + \ldots + a_{n-1}\lambda + a_n .$$

An elementary subgraph of G is a subgraph whose connected component is regular and of degree 1 or 2. In other words, the connected components are single edges and/or cycles.

Theorem 1. ([6]) Let G be a graph and $\psi(G,\lambda)$ be the characteristic polynomial of G, then the coefficients of $\psi(G,\lambda)$ are:

$$(-1)^i a_i = \sum (-1)^{r(H)} 2^{s(H)} ,$$

where the summation is over all elementary subgraphs H of G which have i vertices and $r(H)=n-c$ and $s(H)=m-n+c$, where c is the number of connected components of H, and m, n are the number of edges and vertices of H, respectively.

Corollary 2. The relation between $m(G,k)$ and a_{2k} is as the following:

$$a_{2k} - (-1)^k m(G,k) = \sum (-1)^{r(H)} 2^{s(H)},$$

where the summation is over all elementary subgraphs H of G which have $2k$ vertices and at least one cycle.

Proposition 3. ([6]) By the notation given above we have:

(i) $a_1 = 0$,
(ii) a_2 = the number of edges of G,
(iii) a_3 = twice the number of triangles in G.

In the following we consider a walk and the spectral moments in graph G, see [7] for details.

Definition 4. Let G be a graph. A walk of length k in G is an alternating sequence v_1, e_1, v_2, e_2, …, v_k, e_k, v_{k+1} of vertices and edges such that for any i = 1, 2, …, k the vertices v_i and v_{i+1} are distinct end-vertices of the edge e_i. A closed walk is a walk in which the first and the last vertex are the same.

Let $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ be eigenvalues of $A(G)$. The numbers $S_k(G) = \sum_{i=1}^{n} \lambda_i^k$ are said to be the k–th spectral moment of G. It is well–known that $S_0(G) = n$, $S_1(G) = 0$, $S_2(G) = 2m$ and $S_3(G) = 6t$, where n, m and t denote the number of vertices, edges and triangles of the graph, respectively [7].

Lemma 5. ([7]) The k–th spectral moment of G is equal to the number of closed walks of length k.

In [20, 21] the authors calculated the spectral moments of some graphs and they have ordered them with respect to their spectral moments. Also, in [23] the authors studied the signless Laplacian spectral moments of some graphs and then they ordered the graphs with respect to signless Laplacian spectral moments. In [5, 24] the authors computed the number of 4 and 5–matchings in a graph, and in this paper, we consider the relation between the coefficients of characteristic polynomial and the spectral moments are computed, and then by using this relation the relationship between the coefficients of characteristic polynomial and the coefficients of matching polynomial is determined.

Theorem 6.(**Newton's identity**) Let $\lambda_1(G), \lambda_2(G), ..., \lambda_n(G)$ be the roots of the polynomial $\psi(G,\lambda) = \lambda^n + a_1\lambda^{n-1} + ... + a_{n-1}\lambda + a_n$ with spectral moment S_k. Then

$$a_k = -1/k(S_k + S_{k-1}a_1 + S_{k-2}a_2 + ... + S_1 a_{k-1}).$$

Let F_1, F_2, F_3 and F_4 be a (3, 5, 6)–fullerene, (4, 5, 6)–fullerene, (5, 6, 7)–fullerene and (4, 6, 8)–fullerene, respectively. In [22] the authors computed the spectral moments of this fullerene graphs as in the following:

Theorem 7. The spectral moments of F_1, $S_i(F_1)$, $2 \le i \le 8$, can be computed by the following formulas: $S_2(F_1)=3n$, $S_3(F_1) = 12$, $S_4(F_1) = 15n$, $S_5(F_1) = 180$, $S_6(F_1) = 93n - 60$, $S_7(F_1) = 1932$ and $S_8(F_1) = 639n - 960$.

Theorem 8. The spectral moments of F_2, $S_i(F_2)$, $2 \le i \le 8$, can be computed by the following formulas: $S_2(F_2)=3n$, $S_3(F_2) = 0$, $S_4(F_2) = 15n + 16$, $S_5(F_2) = 80$, $S_6(F_2) = 93n + 96$, $S_7(F_2) = 1120$, $S_8(F_2) = 639n + 400$.

Theorem 9. The spectral moments of F_3, $S_i(F_3)$, $2 \le i \le 8$, can be computed by the following formulas: $S_2(F_3)=3n$, $S_3(F_3) = 0$, $S_4(F_3) = 15n$, $S_5(F_3) = 140$, $S_6(F_3) = 93n - 168$, $S_7(F_3) = 1988$, $S_8(F_3) = 639n - 2464$.

Theorem 10. The spectral moments of F_4, $S_i(F_4)$, $2 \le i \le 8$, can be computed by the following formulas: $S_2(F_4)=3n$, $S_3(F_4) = 0$, $S_4(F_4) = 15n+96$, $S_5(F_4) = 0$, $S_6(F_4) = 93n + 960$, $S_7(F_4) = 0$, $S_8(F_4) = 639n + 8256$.

3. MAIN RESULTS

In this section, we discuss the relationship between the coefficients of characteristic polynomial and the number of 5– and 6– matchings in regular graphs with girth 5 so that every 6–cycle has at most one edge in common with 5–cycles and with other 6–cycles and also any two 5–cycles are at distance at least 2. Then we determine these relations for ***IPR*** (5, 6)–fullerenes, and also we compute the coefficients of the characteristic polynomial of some generalized fullerene graphs.

Theorem 11. Suppose G is an r–regular graph satisfying the above conditions. Then the relation between the tenth coefficient of characteristic polynomial of G and $m(G, 5)$ is the following:

$$a_{10} + m(G,5) = -2\varphi(C_{10}) + \varphi(C_8)nr - 16\varphi(C_8)r + 16\varphi(C_8) - 1/4\varphi(C_6)n^2r^2 - 54\varphi(C_6)r^2$$
$$-13/2\varphi(C_6)nr - 54\varphi(C_6) + 108\varphi(C_6)r + 7\varphi(C_6)nr^2 + 2\varphi(C_5)^2 - 2\varphi(C_5).$$

Proof. By using of Theorem 1, we have:

$$a_{10} = -m(G,5) + \sum_A (-1)^9 2 + \sum_B (-1)^8 2 + \sum_C (-1)^7 2 + \sum_D (-1)^8 4,$$

where A is a 10–cycle, B is a subgraph isomorphic with a 8–cycle and one single edge, C is a subgraph isomorphic with a 6–cycle with two separate edges and D is a subgraph isomorphic with two separate 5–cycles. Now, the values of A, B, C and D are calculated. It is clear that $|A|=\varphi(C_{10})$ and $|B|=\varphi(C_8)(m-8-8(r-2))= \varphi(C_8)(nr/2-8r+8)$. To compute $|C|$ we consider all undesirable cases to have a subgraph isomorphic with C and then subtract these values of all the possible situations. Since all subgraphs isomorphic with C is equal to $\varphi(C_6)$ $(nr/2-6)(nr/2-7)/2$, so if we put $\varphi(C_6)=h$, $\varphi(C_{10})=t$ and $\varphi(C_8)=k$, then $|C|= 1/8hn^2r^2+13/4hnr+27h +27hr^2-54hr-7/2hnr^2$. Also, as it can be observed $|D|= p(p-1)/2$. Therefore

$$a_{10} + m(G,5) = -2t + knr - 16kr + 16k - 1/4hn^2r^2 \\ -54hr^2 - 13/2hnr - 54h + 108hr + 7hnr^2 + 2p^2 - 2p.$$

In the following section, we consider relationship between the twelfth coefficients of characteristic polynomial of a regular graph with consideration of the above conditions. Before the proof of the main result, we need some technical Lemmas.

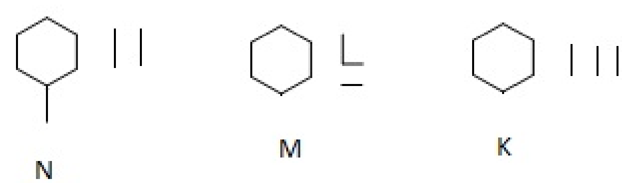


Figure 3. All subgraphs isomorphic with N, M and K.

Lemma 12. Let G be an r–regular graph that above conditions exist for it. Then the number of subgraphs isomorphic with a 6–cycle together with a pendant edge and with two separate edges is equal to:

$$81/2hnr^2 - 33/2hnr^3 - 15hnr - 476h + 160hr^3 - 654hr^2 + 906hr + 3/4hn^2r^3 - 3/2hn^2r^2.$$

Proof. Let N be a subgraph isomorphic with a 6–cycle with a pendant edge and two separate edges, where is depicted in Figure 3. To calculate the number of subgraphs isomorphic with N, first we consider all subgraphs isomorphic with N, that is equal to $6h(r-2)(m-7)(m-8)/2$. Next we consider all of the undesirable cases to have a subgraph isomorphic with N where is shown in Table 1. Therefore, by consideration these values and subtracting all undesirable cases from possible conditions for having a subgraph isomorphic with N we have:

$$|N| = 81/2hnr^2 - 33/2hnr^3 - 15hnr - 476h + 160hr^3 - 654hr^2 + 906hr + 3/4hn^2r^3 - 3/2hn^2r^2.$$

Lemma 13. Let G be an r-regular graph satisfying the above conditions. Then the number of subgraphs isomorphic with a 6–cycles together with a single edge and a path P_3 (where the edge and P_3 are distinct) is equal to:

$$1/4hn^2r^3 + 555hr + 111hr^3 - 420hr^2 + hbr + hbr^3 - 2hbr^2$$
$$-10hnr + 19hnr^2 - 1/4hn^2r^2 - 9hnr^3 - 258h.$$

Proof. Let M be a subgraph isomorphic with a 6–cycle together with a single edge and a path P_3, where is depicted in Figure 3. To calculate $|M|$, the same as previous Lemma, we consider all of the possible cases to have a subgraph isomorphic with M and all adverse conditions that are shown in Table 2. All possible cases is equal to $h(3(r–2)(r–3)+(n–6)r(r–1)/2)(nr/2–8)$, and to obtain adverse conditions, these cases are easily computable and we just compute the cases 8 and 9 in Table 2.

In case 8 (a 6–cycle together with a path P_3 with an edge at the end of this path), first we choose a 6–cycle. Then we consider all the adjacent vertices to 6-cycle, where the number of these vertices is $6(r–2)$. So by a simple check there are $6(r–2)(r–1)(r–2)(2r–2)/2$ ways for selecting the path P_3 with an edge at the end of this path, for the adjacent vertices to 6–cycle. Now we consider all of vertices that are at distance 2 from 6–cycle and we consider the following cases:

Case 1. If this vertex that is at distance 2 from 6–cycle is on a 5–cycle, then we have the following subcases:

Subcase 1.1. If both selected edges to form path P_3 are on 5–cycle, then there are $2(r$-$2)$ ways for selecting the path P_3 with an edge at the end of this path.

Subcase 1.2. If only an edge of P_3 is on 5–cycle, where the number of these edges are equal to $2(r$-$2)$, then there are $2(r$-$2)(2r$-$3)$ ways for selecting the path P_3 with an edge at the end of this path.

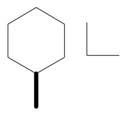
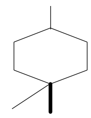
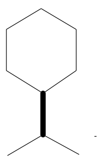
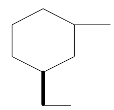
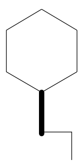
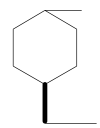
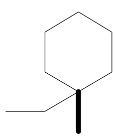
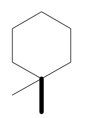
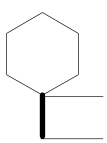
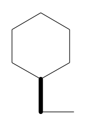
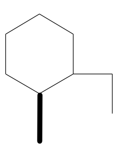
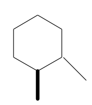
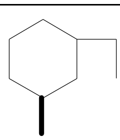
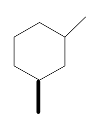
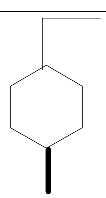
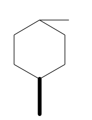
Subcase 1.3. If none of the two edges of path is on 5–cycle, where the number of these edges are equal to $(r–2)(r–3)/2$, then there are $(r–2)(r–3)(2r–2)/2$ ways for selecting the path P_3 with an edge at the end of this path. Finally for the case that the vertex in distance 2 from 6–cycle is on a 5–cycle we have

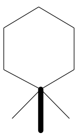
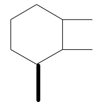
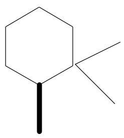
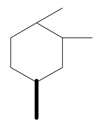
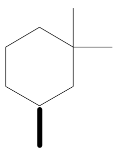
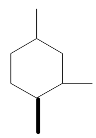
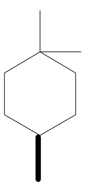
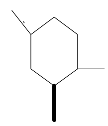
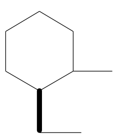
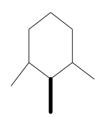
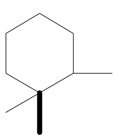
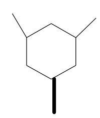
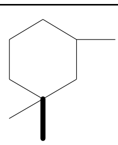
$$b[2r–4+(2r–4)(2r–3)+(r–2)(r–3)(2r–2)/2],$$

where b is the number of edges that are in common with a 6–cycle and a 5–cycle.

Case 2. If the vertex that is at distance 2 from 6–cycle is not on a 5–cycle, where the number of these vertices are equal to $6(r–1)(r–2)–2b$, then there are $(r–1)(2r–3)$ + $(r–1)(r–2)(2r–2)/2$ ways for selecting the path P_3 with an edge at the end of this path.

Table 1. All of the undesirable situations to have a 6–cycle with a pendant edge and with two separate edges and their numbers.

	$3h(r-2)\left(-21r^2+49r-28+nr^2-nr\right)$		$6h(r-2)^2(r-3)$
	$3h(r-2)^2(r-1)$		$6h(r-2)^2(r-1)$
	$6h(r-2)(r-1)^2$		$6h(r-2)^2(r-1)$
	$6h(r-2)(r-1)(r-3)$		$3h(r-2)(r-3)(nr-16r+16)$
	$6h(r-2)(r-1)(r-3)$		$3h(r-2)(r-1)(nr-16r+16)$
	$6h(r-2)^2(r-1)$		$3h(r-2)^2(nr-16r+16)$
	$6h(r-2)^2(r-1)$		$3h(r-2)^2(nr-16r+16)$
	$6h(r-2)^2(r-1)$		$\frac{3}{2}h(r-2)^2(nr-16r+16)$

	$3\,h(r-2)(r-3)(r-4)$		$6\,h\,(r-2)^3$
	$3\,h\,(r-2)^2\,(r-3)$		$6\,h\,(r-2)^3$
	$3\,h\,(r-2)^2\,(r-3)$		$6\,h\,(r-2)^3$
	$3\,h\,(r-2)^2\,(r-3)$		$6\,h\,(r-2)^3$
	$6\,h\,(r-2)^2\,(r-1)$		$6\,h\,(r-2)^3$
	$6\,h\,(r-2)^2\,(r-3)$		$2\,h\,(r-2)^3$
	$6\,h\,(r-2)^2\,(r-3)$		

Finally, for the case that the vertex in distance 2 from 6–cycle is not on a 5–cycle, there are

$$b(2r-4+(2r-4)(2r-3)+(r-2)(r-3)(2r-2)/2)+$$
$$(6(r-1)(r-2)-2b)((r-1)(2r-3)+(r-1)(r-2)(2r-2)/2)$$

ways for selecting the path P_3 with an edge at the end of this path. Therefore, to calculate case 8 in Table 2 we have:

$$\begin{aligned} &h[6(r-2)(r-1)(r-2)(2r-2)/2+b(2r-4+(2r-4)(2r-3)\\ &\quad+(r-2)(r-3)(2r-2)/2)+(6(r-1)(r-2)-2b)((r-1)(2r-3)\\ &\quad+(r-1)(r-2)(2r-2)/2)+(n-6-6(r-2)-6(r-1)(r-2))r(r-1)(2r-2)/2]\\ &\quad=h(nr^3-2nr^2+nr-br^3+2br^2-br+84r^2-24r^3-96r+36). \end{aligned}$$

In case 9 Table 2, (a 6–cycle together with a path P_3 and an edge on middle vertex of P_3), we first select a 6–cycle and then a path P_3 of all the vertices except vertices of 6-cycle. For the vertices that are at distance 1 from 6–cycle, where the number of these vertices are 6(*r*–2), there are 6((*r*–2)(*r*–1)(*r*–2)/2)(*r*–3) ways to choose a path P_3 such that there is an edge on the middle vertex. For other vertices, where the number of these vertices are *n*–6–6(*r*–2), there are (*n*–6–6(*r*–2))*r*(*r*–1)(*r*–2)/2) ways to choose a path P_3 such that there is an edge on middle vertex. Therefore, there are *h*(6(*r*–2)(*r*–1)(*r*–2)/2)(*r*–3) + (*n*–6–6(*r*–2))*r*(*r*–1)(*r*–2)/2) ways to choose case 9 of Table 2. Finally, after calculating all adverse conditions in this Table, we have:

$$\begin{aligned} |M| &= 1/4hn^2r^3+555hr+111hr^3-420hr^2+hbr+hbr^3-2hbr^2\\ &\quad-10hnr+19hnr^2-1/4hn^2r^2-9hnr^3-258h. \end{aligned}$$

Lemma 14. Let *G* be an *r*–regular graph with the above conditions. Then the number of subgraphs isomorphic with a 6–cycle together with three separate edges is equal to:

$$\begin{aligned} &-147hr+59/6hnr^3-5/2hnr^2-44/3hnr+2hbr^2-hbr\\ &+136h-hbr^3-57hr^3+126hr^2-hn^2r^3+1/48hn^3r^3+7/8hn^2r^2. \end{aligned}$$

P**roof.** Let *K* be a subgraph isomorphic with a 6–cycle and three separate edges, where is depicted in Figure 3. To calculate |*K*|, we must consider all the undesirable cases for having a subgraph isomorphic with *K*, that is shown in Table 3 and then we subtract these values of all the possible situations to have a subgraph isomorphic with *K*. Notice that all subgraphs isomorphic with *K* is equal to *h*(*m*-6)(*m*-7)(*m*-8)/6, so we must find a formula for all adverse conditions . In this Table all of values in front of figures are easily calculated, and with putting up values of Lemmas 12 and 13 we obtain:

$$\begin{aligned} |K| &= -147hr+59/6hnr^3-5/2hnr^2-44/3hnr+2hbr^2-hbr\\ &\quad+136h-hbr^3-57hr^3+126hr^2-hn^2r^3+1/48hn^3r^3+7/8hn^2r^2. \end{aligned}$$

Theorem 15. Suppose *G* is an *r*–regular graph satisfying the above conditions. Then the relationship between the twelfth coefficients of characteristic polynomial of *G* and *m*(*G*, 6) is stated in the following:

$$a_{12} - m(G,6) = -4a - 2e - 88/3hnr - 2hbr + 59/3hnr^3 - 5hnr^2 + 7/4hn^2r^2 - 72k$$
$$+ 4hbr^2 - 2hbr^3 - 68kr^2 + 20t + 1/24hn^3r^3 - 20p^2 - 2hn^2r^3 - 4kr^3$$
$$- 20tr + 9knr^2 - 1/4kn^2r^2 - 17/2knr - 294hr + pnr + 20p^2r + 270h$$
$$+ 252hr^2 - 114hr^3 + 144kr - 20pr + tnr + 20p + 2h^2 - p^2nr,$$

where $k=\varphi(C_8)$, $e=\varphi(C_{12})$, $t=\varphi(C_{10})$, $p=\varphi(C_5)$, $h=\varphi(C_6)$, a is the number of edges common to two 6-cycles and b is the number of edges that are in common with a 6–cycle and a 5–cycle.

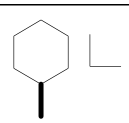
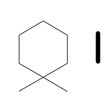
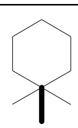
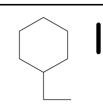
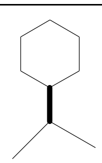
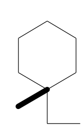
Proof. By Theorem 1 we have:

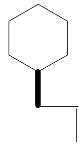
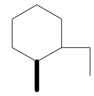
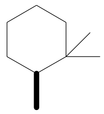
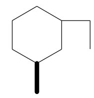
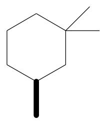
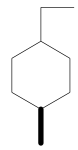
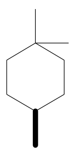
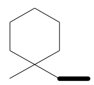
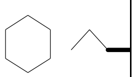
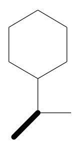
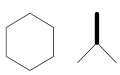
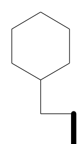
$$a_{12} = m(G,6) + \sum_A (-1)^{10} 2 + \sum_B (-1)^{11} 2 + \sum_C (-1)^9 2 + \sum_D (-1)^8 2 + \sum_E (-1)^9 4 + \sum_F (-1)^{10} 4,$$

where A is a subgraph isomorphic with a 10–cycle and a single edge, B is a subgraph isomorphic with a 12–cycle, C is a subgraph isomorphic with a 8–cycle and two separate edges, D is a subgraph isomorphic to 6–cycle together with three separate edges, E is a subgraph isomorphic to two separate 5–cycles with one single edge and F is a subgraph isomorphic with two separate 6–cycles. It is easy to see that $|A|= t(nr/2-10r+10)$ and $|B|=e$. To calculate $|C|$, we consider all of the possible cases to have a subgraph isomorphic with a 8–cycle with two separate edges and all of the undesirable situations, and so we obtain:

$$|C| = k/2(m-8)(m-9) - k(2(r-2)^2(r-1) + (n-8r+8)r(r-1)/2)$$
$$- 4k(r-2)(r-3) - 8k(r-2)(r-1) - 28k(r-2)^2 - 8k(r-2)(nr/2 - 9r + 9)$$
$$= 1/8kn^2r^2 + 17/4knr + 36k + 2kr^3 + 34kr^2 - 72kr - 9/2knr^2.$$

Table 2. All of the undesirable situations to have a 6–cycle with a single edge and a path P_3 and their numbers.

	$3h(r-2)(-21r^2+49r-28+nr^2-nr)$		$\frac{3}{2}h(r-2)(r-3)(rn-16r+16)$
	$3h(r-2)(r-3)(r-4)$		$3h(r-2)(r-1)(rn-16r+16)$
	$3h(r-2)^2(r-1)$		$6h(r-2)(r-1)(r-3)$

	$6h(r-2)(r-1)^2$		$6h(r-2)^2(r-1)$
	$3h(r-2)^2(r-3)$		$6h(r-2)^2(r-1)$
	$3h(r-2)^2(r-3)$		$6h(r-2)^2(r-1)$
	$3h(r-2)^2(r-3)$		$3h(r-2)(r-3)(r-1)$
	$-h(-36+96r-nr+2nr^2-nr^3+24r^3-84r^2+br-2br^2+br^3)$		$6h(r-2)^2(r-1)$
	$\frac{1}{2}h(r-2)(r-1)(-24r+36+rn)$		$6h(r-2)(r-1)^2$

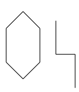
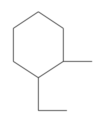
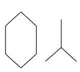
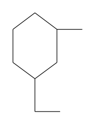
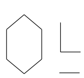
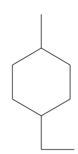
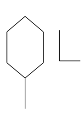
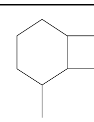
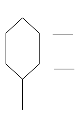
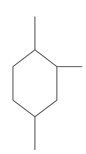
On the other hand, by Lemma 14,

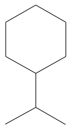
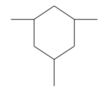
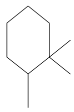
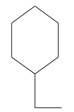
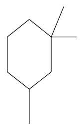
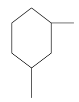
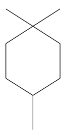
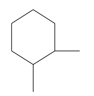
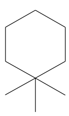
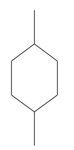
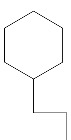
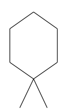
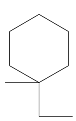
$$|D|=-147hr+59/6hnr^3-5/2hnr^2-44/3hnr+2hbr^2-hbr$$
$$+136h-hbr^3-57hr^3+126hr^2-hn^2r^3+1/48hn^3r^3+7/8hn^2r^2.$$

Let p be the number of 5–cycles that are satisfied in above conditions, i.e. every 6–cycle has at most one edge in common with a 5–cycle and the other 6–cycles and also any two 5–cycles has distance of at least 2. Then, it is clear that $|E|=p(p-1)/2(nr/2-10r+10)$. Now let a be the number of edges common to two 6–cycles, then $|F|=h(h-1)/2-a$. Therefore,

$$
\begin{aligned}
a_{12} - m(G,6) &= 2t(nr/2 - 10r + 10) - 2e - 2(1/8kn^2r^2 + 17knr/4 + 36k + 2kr^3 + 34kr^2 \\
&\quad - 72kr - 9knr^2/2) + 2(-147hr + 59/6hnr^3 - 5/2hnr^2 - 44/3hnr + 2hbr^2 \\
&\quad - hbr + 136h - hbr^3 - 57hr^3 + 126hr^2 - hn^2r^3 + 1/48hn^3r^3 + 7/8hn^2r^2) \\
&\quad - 4(p(p-1)/2(nr/2 - 10r + 10)) + 4(h(h-1)/2 - a) \\
&= -4a - 2e - 88/3hnr - 2hbr + 59/3hnr^3 - 5hnr^2 + 7/4hn^2r^2 - 72k \\
&\quad + 4hbr^2 - 2hbr^3 - 68kr^2 + 20t + 1/24hn^3r^3 - 20p^2 - 2hn^2r^3 - 4kr^3 \\
&\quad - 20tr + 9knr^2 - 1/4kn^2r^2 - 17/2knr - 294hr + pnr + 20p^2r + 270h \\
&\quad + 252hr^2 - 114hr^3 + 144kr - 20pr + tnr + 20p + 2h^2 - p^2nr.
\end{aligned}
$$

Table 3. All of the undesirable situations to have a 6-cycle with three separate edges and their numbers.

	$-12hr^3 + 42hr^2 - 48hr + 18h + \frac{1}{2}hnr^3 - hnr^2 + \frac{1}{2}hnr$		$6h(r-2)^2(r-1)$
	$-4hr^3 + 18hr^2 - 26hr + 12h + \frac{1}{6}hnr^3 - \frac{1}{2}hnr^2 + \frac{1}{3}hnr$		$6h(r-2)^2(r-1)$
	$\frac{1}{4}hn^2r^3 + 555hr + 111hr^3 - 420hr^2 + hbr + hbr^3 - 2hbr^2 - 10hnr + 19hnr^2 - \frac{1}{4}hn^2r^2 - 9hnr^3 - 258h$		$6h(r-2)^2(r-1)$
	$3h(r-2)\left(-21r^2 + 49r - 28 + nr^2 - nr\right)$		$6h(r-2)^3$
	$\frac{81}{2}hnr^2 - \frac{33}{2}hnr^3 - 15hnr - 476h + 160hr^3 - 654hr^2 + 906hr + \frac{3}{4}hn^2r^3 - \frac{3}{2}hn^2r^2$		$6h(r-2)^3$

	$3h(r-1)(r-2)^2$		$2h(r-2)^3$
	$3h(r-3)(r-2)^2$		$3h(r-1)(r-2)(nr-16r+16)$
	$3h(r-3)(r-2)^2$		$3h(r-2)^2(nr-16r+16)$
	$3h(r-3)(r-2)^2$		$3h(r-2)^2(nr-16r+16)$
	$h(r-3)(r-2)(r-4)$		$\frac{3}{2}h(r-2)^2(nr-16r+16)$
	$6h(r-1)^2(r-2)$		$\frac{3}{2}h(r-2)(r-3)(nr-16r+16)$
	$6h(r-3)(r-2)(r-1)$		

In following, suppose G is an ***IPR*** (5, 6)–fullerene such that any two pentagons are at distance at least 2. In [13] the authors calculated some of the coefficients of characteristic polynomial of G. Now, in this paper by using these coefficients and by using of Theorems 11 and 15 we calculate the 5, 6-matchings in G.

Theorem 16. Let G be an ***IPR*** (5, 6)–fullerene such that satisfying the above conditions. Then we have:

$$m(G,5) = 3543/10n - 12 + 1719/64n^3 - 2499/16n^2 - 135/64n^4 + 81/1280n^5.$$

Proof. By using of Theorem 11 we have:

$$a_{10} + m(G,5) = -2t + knr - 16kr + 16k - 1/4hn^2r^2$$
$$-54hr^2 - 13/2hnr - 54h + 108hr + 7hnr^2 + 2p^2 - 2p.$$

On the other hand by [13] we have:

$$a_{10} = -81/1280n^5 + 135/64n^4 - 1791/64n^3 + 3207/16n^2 - 9003/10n + 2556.$$

Also we have, r=3, $\varphi(C_{10})=a=3n/2-60$, $\varphi(C_8)=0$, $\varphi(C_5)=12$ and $\varphi(C_6)=n/2-10$. Therefore, $m(G,5) = 3543/10n - 12 + 1719/64n^3 - 2499/16n^2 - 135/64n^4 + 81/1280n^5$.

Theorem 17. Let G be an ***IPR*** (5, 6)–fullerene such that satisfies the above conditions. Then we have:

$$m(G,6) = -7607/4n - 10770 + 146177/160n^2 - 21339/128n^3$$
$$+ 4113/256n^4 - 405/512n^5 + 81/5120n^6.$$

Proof. By using of Theorem 15 we have:

$$m(G,6) = a_{12} - (-4a - 2e - 88/3hnr - 2hbr + 59/3hnr^3 - 5hnr^2 + 7/4hn^2r^2 - 72k$$
$$+ 4hbr^2 - 2hbr^3 - 68kr^2 + 20t + 1/24hn^3r^3 - 20p^2 - 2hn^2r^3 - 4kr^3$$
$$- 20tr + 9knr^2 - 1/4kn^2r^2 - 17/2knr - 294hr + pnr + 20p^2r + 270h$$
$$+ 252hr^2 - 114hr^3 + 144kr - 20pr + tnr + 20p + 2h^2 - p^2nr).$$

On the other hand, by [13] and by Newton's identity we have:

$$a_{12} = -31899/4n + 25970 + 240017/160n^2 - 25227/128n^3$$
$$+ 4257/256n^4 - 405/512n^5 + 81/5120n^6.$$

Also, in an IPR (5,6)–fullerene we have, $e = \varphi(C_{12})=0$, $t = \varphi(C_{10})=a=3n/2-60$, $k=\varphi(C_8)=0$, $p=\varphi(C_5)=12$, $h = \varphi(C_6) = n/2-10$ and b = the number of edges are common to 6–cycles and 5–cycles = 60. Therefore,

$$m(G,6) = -7607/4n - 10770 + 146177/160n^2 - 21339/128n^3$$
$$+ 4113/256n^4 - 405/512n^5 + 81/5120n^6.$$

In the following we consider all of the generalized fullerene graphs that were defined in this paper and the coefficients of characteristic polynomial of these graphs are calculated.

Theorem 18. The coefficients of characteristic polynomial of F_1, $a_i(F_1)$, for i =1, 2, 3, …, 8 are: $a_1 = 0$, $a_2 = -3n/2$, $a_3 = -4$, $a_4 = 9/8n^2 - 15n/4$, $a_5 = 6n - 36$, $a_6 = -9n^3/16 + 45n^2/8 - 31/2n + 18$, $a_7 = -9n^2/2 + 69n - 276$, $a_8 = 27n^4/128 - 135n^3/32 + 969n^2/32 - 855n/8 + 264$.

Proof. Apply Theorems 7−10 and Newton's identity.

Theorem 19. The coefficients of characteristic polynomial of F_2, $a_i(F_2)$, for i =1, 2, 3, …, 8 are: $a_1 = 0$, $a_2 = -3n/2$, $a_3 = 0$, $a_4 = 9n^2/8 - 15n/4 - 4$, $a_5 = -16$, $a_6 = -9n^3/16 + 45n^2/8 - 19n/2 - 16$, $a_7 = 24n - 160$, $a_8 = 27n^4/128 - 135n^3/32 + 825n^2/32 - 327n/8 - 42$.

Theorem 20. The coefficients of characteristic polynomial of F_3, $a_i(F_3)$, for i =1, 2, 3, …, 8 are: $a_1 = 0$, $a_2 = -3n/2$, $a_3 = 0$, $a_4 = 9n^2/8 - 15n/4$, $a_5 = -28$, $a_6 = -9n^3/16 + 45n^2/8 - 31n/2 + 28$, $a_7 = 42n - 284$, $a_8 = 27n^4/128 - 135n^3/32 + 969n^2/32 - 975n/8 + 308$.

Theorem 21. The coefficients of characteristic polynomial of F_4, $a_i(F_4)$, for i =1, 2, 3, …, 8 are: $a_1 = 0$, $a_2 = -3n/2$, $a_3 = 0$, $a_4 = 9n^2/8 - 15n/4 - 24$, $a_5 = 0$, $a_6 = -9n^3/16 + 45n^2/8 + 41n/2 - 160$, $a_7 = 0$ and $a_8 = 27n^4/128 - 135n^3/32 + 105n^2/32 + 2001n/8 - 744$.

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