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Matchings in Tetrameric 1, 3-Adamantane

Fatemeh Taghvaee[1*] **and Gholam Hossein Fath-Tabar**[2]

[1]*Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan 87317-53153, I. R. Iran.*
[2]*Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan 87317-53153, I. R. Iran.*
[*]*Corresponding author E-mail: taghvaei19@yahoo.com*

Abstract

Suppose G is a graph, $A(G)$ its adjacency matrix, and $\varphi(G,\lambda)=\sum_{i=0}^{n}a_i\lambda^{n-i}$ is the characteristic polynomial of G. The polynomial $M(G,x)=\sum_{k\geq 0}(-1)^k m(G,k)x^{n-2k}$, is called the matching polynomial of G, where $m(G,k)$ is the number of $k-$matchings in G. In this paper, we consider tetrameric 1, 3-adamantane, $TA(N)$, and determine some coefficients of characteristic polynomial and matching polynomial of $TA(N)$.

Keywords: *Characteristic polynomial, matching polynomial, spectral moment, tetrameric 1, 3-adamantane.*
2010 Mathematics Subject Classification: *05C50,15A18*

1. Introduction

Suppose G is a simple graph with n vertices and m edges. The adjacency matrix of G is a square $n\times n$ matrix A such that A_{ij} is 1 when there is an edge from v_i to v_j and zero when there is no edge. The characteristic polynomial of G, denoted by $\varphi(G,\lambda)$, is defined as:

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

The roots of the characteristic polynomial are called the eigenvalues of G and the eigenvalues together with their multiplicities form the spectrum of G. A matching in a graph G is a set of its edges such that no two edges of this set have a vertex in common. The matching polynomial of G is defined as:

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

where $m(G,k)$ is the number of $k-$matchings in G [9]. It is clear that $m(G,1)=m$ and $m(G,k)=0$ for $k>\lfloor\frac{n}{2}\rfloor$ or $k<0$. The matching polynomial is an important concept in Combinatorics and Theoretical Chemistry [7, 8, 10, 11]. A walk of length k in a graph 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 $i=1,2,\ldots,k$, 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 vertices are the same.
Let $\lambda_1,\ldots,\lambda_n$ be the eigenvalues of $A(G)$. The numbers $S_k(G)=\sum_{i=1}^{n}\lambda_i^k$ are called the $k-$th spectral moment of G. It is easy to see 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 G, respectively [4].
Strightforward computations yield that $|V(TA(N))|=10N$ and $|E(TA(N))|=13N-1$. Some authors computed the 4 and 5-matchings in a graph [2, 15]. In this paper we consider a tetrameric 1, 3-adamantane, $TA(N)$, and we find the spectral moments of this graph and then by these spectral moments we compute the number of the $k-$matchings in $TA(N)$ for $N\geq 3$ and $k=2,3,4$.

2. Preliminaries

Our terminology and notations are mostly standard and are taken from Biggs [3]. Suppose G is a graph with n vertices, m edges and with adjacency matrix $A(G)$. The characteristic polynomial of G, $\varphi(G,\lambda)$, is defined as

$$\varphi(G,\lambda)=\lambda^n+a_1\lambda^{n-1}+\cdots+a_n.$$

An elementary subgraph of G is a subgraph, each of whose connected component is regular and has degree 1 or 2. In other words, the connected components are single edges or a cycle. The following theorems of Biggs [3] is crucial throughout this paper.

Email addresses: **, taghvaei19@yahoo.com (Fatemeh Taghvaee), fathtabar@kashanu.ac.ir (Gholam Hossein Fath-Tabar)**

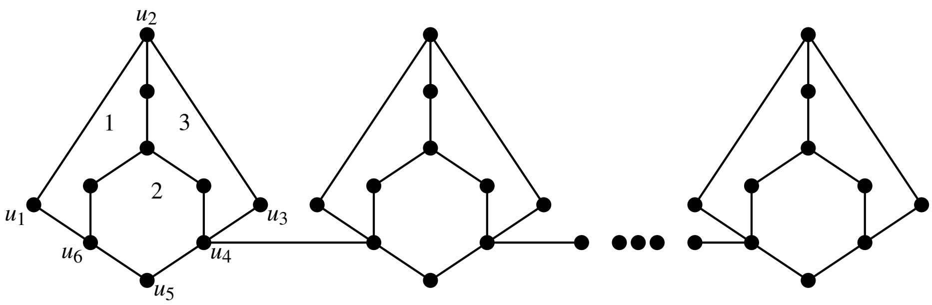

Figure 1.1: The Tetrameric 1, 3-adamantane $TA(N)$.

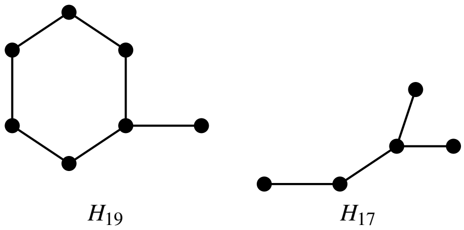

Figure 2.1: The subgraphs H_{19} and H_{17}.

Theorem 2.1. *Let G be a graph and $\varphi(G,\lambda)$ be the characteristic polynomial of G. Then $(-1)^i a_i = \sum(-1)^{r(H)}2^{s(H)}$, where the summation is taken 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.*

Theorem 2.2. *Let G be a graph with characteristic polynomial $\varphi(G,\lambda)$. Then*

1. *$a_1 = 0$,*
2. *a_2=the number of edges of G,*
3. *a_3=twice the number of triangles in G.*

Throughout this paper, denote by P_n, C_n, S_n and U_n a path, a cycle, a star with n verices and a graph obtained from C_{n-1} by attaching a vertex of degree 1 to one vertex of C_{n-1}, respectively. Suppose F and G are graphs. An $F-$subgraph of G is a subgraph isomorphic to the graph F. The number of all $F-$subgraphs of G is denoted by $\phi_G(F)$. For the sake of completeness, we mention here three lemmas from Cvetković et al [4], Wu and Liu [16].

Lemma 2.3. *The $k-$th spectral moment of G is equal to the number of closed walks of length k in G.*

Lemma 2.4. *For any graph G, we have*

1. $S_4(G) = 2\phi(P_2)+4\phi(P_3)+8\phi(C_4)$,
2. $S_5(G) = 30\phi(C_3)+10\phi(U_4)+10\phi(C_5)$,
3. $S_6(G) = 2\phi(P_2)+12\phi(P_3)+6\phi(P_4)+12\phi(S_4)+12\phi(U_5)+36\phi(B_4)+24\phi(B_5)+24\phi(C_3)+48\phi(C_4)+12\phi(C_6)$.

Lemma 2.5. *For any graph G, we have*

1. $S_7(G) = 126\phi(C_3)+84\phi(H_1)+28\phi(H_7)+14\phi(H_5)+14\phi(H_6)+112\phi(H_3)+42\phi(H_{15})+28\phi(H_8)+70\phi(C_5)+14\phi(H_{18})+14\phi(C_7)$,
2. $S_8(G) = 2\phi(P_2)+28\phi(P_3)+32\phi(P_4)+8\phi(P_5)+72\phi(K_{1,3})+16\phi(H_{17})+48\phi(K_{1,4})+168\phi(C_3)+64\phi(H_1)+464\phi(H_3)+384\phi(H_4)+96\phi(H_{15})+96\phi(H_{10})+48\phi(H_{11})+80\phi(H_{12})+32\phi(H_{16})+264\phi(C_4)+24\phi(H_9)+112\phi(H_2)+16\phi(H_{23})+16\phi(H_{20})+16\phi(H_{21})+32\phi(H_{22})+32\phi(H_{13})+32\phi(H_{14})+528\phi(K_4)+96\phi(C_6)+16\phi(H_{19})+16\phi(C_8)$.

Some authors applied above formula to calculate the spectral moments of some graphs. They also gave an ordering of these graphs with respect to spectral moments [12]. Also some authors found signless Laplacian spectral moments of graphs and then they order some graphs with respect to them [13, 14].

Theorem 2.6. *(Newtonś identity) Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the roots of the polynomial $\varphi(G,\lambda) = \lambda^n + a_1\lambda^{n-1} + \cdots + a_n$ with spectral moment S_k. Then*

$$a_k = \frac{-1}{k}(S_k + S_{k-1}a_1 + \ldots + S_1 a_{k-1}).$$

3. Main Results

In this section, first we find the spectral moments of $TA(N)$, for $k = 1,2,3,\ldots,8$ and then by Newtonś identity compute the coefficients of characteristic polynomial and matching polynomial in $TA(N)$ for $N \geq 3$.

Theorem 3.1. *In a tetrameric 1, 3-adamantane $TA(N)$ we have*

$$\phi(P_2) = 13N-1, \quad \phi(P_3) = 24N-6, \quad \phi(P_4) = 39N-15, \quad \phi(P_5) = 67N-32.$$

Proof. It is easy to see that $\phi(P_2) = m = 13N-1$. In a tetrameric 1, 3-adamantane with $10N$ vertices, there are $2N+2$ vertices of degree 3, $6N$ vertices of degree 2 and $2N-2$ vertices of degree 4. So $\phi(P_3) = 24N-6$.
To calculate $\phi(P_4)$, we select an edge e. There are three type of edges in $TA(N)$. The first type edges are those with an end vertex of degree 2 and another of degree 3. The number of these edges is equal to $6N+6$. The second type of edges are those with an end vertex of degree 2 and another of degree 4. The number of these edges is equal to $6N-6$. The third type of edges are those both end vertices have degree 4. It is easy to see that the number of these edges is equal to $N-1$. Now if e is an edge of the first type, then the number of subgraphs isomorphic to P_4 is equal to $2(6N+6)$. If e is an edge of the second type, then the number of subgraphs isomorphic to P_4 is equal to $3(6N-6)$ and if e is an edge of the third type, then the number of subgraphs isomorphic to P_4 is equal to $9(N-1)$. Thus $\phi(P_4) = 39N-15$.
To calculate $\phi(P_5)$, we select a vertex v as the middle vertex of $\phi(P_5)$. If v is a vertex of degree 3, then the number of subgraphs isomorphic to $\phi(P_5)$ is equal to $6N+6$. Suppose that v is a vertex of degree 2. Then by a simple calculation we have $\phi(P_5) = 37N-14$. If v is a vertex of degree 4, then $\phi(P_5) = 24N-24$. Therefore $\phi(P_5) = 67N-32$. □

Theorem 3.2. *The spectral moments of $TA(N)$, for $k = 1,2,3,\dots,8$ can be computed as the followings:*

$$S_1(TA(N)) = 0, \quad S_2(TA(N)) = 26N-2, \quad S_3(TA(N)) = 0,$$

$$S_4(TA(N)) = 122N-26, \quad S_5(TA(N)) = 0, \quad S_6(TA(N)) = 716N-236,$$

$$S_7(TA(N)) = 0, \quad S_8(TA(N)) = 4690N-2010.$$

Proof. It is easy to see that $S_1(TA(N)) = 0$. Also since $m(TA(N)) = 13N-1$ and since a tetrameric 1, 3-adamantane is triangle free, $S_3(TA(N)) = 0$. Now we compute the forth spectral moment of $TA(N)$. By using Theorem 2.2 and Lemma 2.2 we have

$$S_4(TA(N)) = 26N-2+4(24N-6) = 122N-26.$$

Since $\phi(C_3) = \phi(C_5) = 0$, $S_5(TA(N)) = 0$. To compute $S_6(TA(N))$ it is easy to check that in $TA(N)$, $\phi(K_{1,3}) = 10N-6$ and so $S_6(TA(N)) = 716N-236$. According to the structure of the tetrameric 1, 3-adamantane and by Lemma 2.5, we have $S_7(TA(N)) = 0$. To calculate the eighth spectral moment of $TA(N)$, we must calculate the number of subgraphs isomorphic to $K_{1,4}$, C_8, H_{17} and H_{19}, where the last two subgraphs are shown in Figure 2.1 and the number of other subgraphs mentioned in Lemma 2.5 is equal to 0. To have a subgraph isomorphic to H_{17}, we select an edge $e = uv$ such that the degree of u is at least 2 and degree of v is at least 3. If e is an edge of the first type, then $\phi(H_{17}) = 6N+6$. While if e is an edge of the second type, then $\phi(H_{17}) = 18N-18$ and otherwise $\phi(H_{17}) = 18N-18$. So in a tetrameric 1, 3-adamantane we have $\phi(H_{17}) = 42N-30$. A simple verification shows that the number of subgraphs isomorphic to H_{19} is equal to $18N-6$ and also $\phi(K_{1,4}) = 2N-2$. Therefore by Lemma 2.5 we have $S_8(TA(N)) = 4690N-2010$. □

Theorem 3.3. *The coefficients of characteristic polynomial of $TA(N)$, for $i = 1,2,3,\dots,8$ are as following:*

$$\begin{aligned}
a_1(TA(N)) &= 0, \ a_2(TA(N)) = -13N+1, \ a_3(TA(N)) = 0,\\
a_4(TA(N)) &= \frac{169N^2}{2} - \frac{87N}{2} + 7, a_5(TA(N)) = 0,\\
a_6(TA(N)) &= \frac{-1445N}{6} + 46 + 481N^2 - \frac{2197N^3}{6}, \ a_7(TA(N)) = 0,\\
a_8(TA(N)) &= \frac{-18205N}{12} + 315 + \frac{72107N^2}{24} - \frac{35321N^3}{12} + \frac{28561N^4}{24}.
\end{aligned}$$

Proof. By Theorem 2.1 and Newtonś identity we can compute the coefficients of characteristic polynomial of a tetrameric 1, 3-adamantane. It is easy to check that $a_1 = a_3 = a_5 = a_7 = 0$. Since $S_2(TA(N)) = 26N-2$, $a_2(TA(N)) = -13N+1$. Also since $S_4(TA(N)) = 122N-26$ and $S_6(TA(N)) = 716N-236$, thus $a_4(TA(N)) = \frac{169N^2}{2} - \frac{87N}{2} + 7$ and $a_6(TA(N)) = \frac{-1445N}{6} + 46 + 481N^2 - \frac{2197N^3}{6}$. Similarly the eighth coefficients of characteristic polynomial of $TA(N)$ can be calculated. □

In the following by Theorems 2.1 and 2.2 we can compute the coefficients of matching polynomial of $TA(N)$, $m(TA(N),k)$, for $k = 2,3,4$ and $N \geq 3$.

Theorem 3.4. *In a tetrameric 1, 3-adamantane, we have:*

$$\begin{aligned}
m(TA(N),2) &= \frac{169N^2}{2} - \frac{87N}{2} + 7,\\
m(TA(N),3) &= \frac{1397N}{6} - 46 - 481N^2 + \frac{2197N^3}{6},\\
m(TA(N),4) &= \frac{-17029N}{12} + 303 + \frac{69611N^2}{24} - \frac{35321N^3}{12} + \frac{28561N^4}{24}.
\end{aligned}$$

Proof. We have $a_4 = \sum(-1)^{r(H)}2^{s(H)}$, where H is an elementary subgraph with 4 vertices. Since there is one elementary subgraph with 4 vertices, $a_4 = m(TA(N),2)) = \frac{1397N}{6} - 46 - 481N^2 + \frac{2197N^3}{6}$. To calculate $m(TA(N),3)$ again by Theorem 2.1 we have

$$a_6 = \sum_A(-1)^3 + \sum_B(-1)^5 2 = -m(TA(N),3) - 2\phi(C_6),$$

where A and B are the subgraphs isomorphic to three separate edges and a 6-cycle, respectively. Due to the structure of a tetrameric 1, 3-adamantane, we have $\phi(C_6) = 4N$ and thus by Theorem 3.3

$$m(TA(N),3) = -a_6 - 8N = \frac{1397N}{6} - 46 - 481N^2 + \frac{2197N^3}{6}.$$

Now we compute the number of 4-matchings in $TA(N)$. We have

$$a_8 = \sum_A (-1)^4 + \sum_B (-1)^6 2 + \sum_C (-1)^7 2 = m(TA(N),4) + 2|B| - 2\phi(C_8),$$

where A, B and C are the four separate edges, a 6-cycle with a single edge and a 8-cycle, respectively. It is easy to see that $|C| = \phi(C_8) = 3N$. Now we calculate the number of subgraphs isomorphic to B. We consider part 1 of $TA(N)$, Figure 1.1. For the first 6-cycle, there are $m-9$ ways to choose a single edge. For each of the second and third 6-cycle there are $m-10$ ways to choose a single edge. Also for the forth 6-cycle, that is $u_1u_2u_3u_4u_5u_6u_1$, there are $m-10$ ways to choose a single edge. Thus for the first part of $TA(N)$ we have, $|B| = 4m-39$. Similarly for the $N-$th part of $TA(N)$ we have, $|B| = 4m-39$. For each of the $(N-2)$ middle part of $TA(N)$ there are in total $4m-42$ ways to select a 6-cycle with a single edge. Finally by putting $m = 13N-1$ we have, $|B| = 2(4m-39)+(N-2)(4m-42) = 52N2-46N+6$. Therefore

$$m(TA(N),4) = \frac{-17029N}{12} + 303 + \frac{69611N^2}{24} - \frac{35321N^3}{12} + \frac{28561N^4}{24}.$$

This completes the proof. □

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