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On the Eigenvalues of Rhomboidal $C_4C_8(R)[n,n]$ Nanotori

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ABSTRACT

A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. It can cover either a cylinder or a torus. In this paper, we determine the adjacency spectrum of rhomboidal C_4C_8 tori. We also give lower and upper bounds for a chemical quantity, namely Estrada index, for a C_4C_8 net.

1. INTRODUCTION

For group theory notation and terminology not given here, we refer to [9] and for algebraic graph theory notation and terminology, we follow [12]. Let $\Gamma = (V(\Gamma), E(\Gamma))$ be a simple connected graph with vertex and edge sets $V(\Gamma)$ and $E(\Gamma)$, respectively. For two vertices u and v of a graph Γ, we denote $u \sim v$ when u and v are *adjacent*. Also, for every $u \in V(\Gamma)$, we denote the set of all adjacent vertices of u with $N(u)$. In chemical graphs, each vertex represents an atom of the molecule, and covalent bonds between atoms are represented by an edge between the corresponding vertices. This shape derived from a chemical compound called the molecular graph, and can be a path, a tree, or in general a graph. A C_4C_8 net ($TUC_4C_8(R)[m,n]$ nanotube) is a *trivalent* decoration made by alternating 4-cycles and 8-cycles. It can cover a cylinder or a torus. The rhomboidal C_4C_8 tori is a molecular graph which introduced by Diudea and John in [7] and [8].

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The *adjacency matrix* of a given graph Γ is the $|V(\Gamma)| \times |V(\Gamma)|$ matrix $A = A(\Gamma) = (a_{ij})$ whose entries a_{ij} are given by

$$a_{ij} = \begin{cases} 1 & v_i \sim v_j \\ 0 & otherwise \end{cases} .$$

The *spectrum* of this graph is the multi set of eigenvalues of its adjacency matrix, the roots of $\det(\lambda I - A) = 0$. If $\lambda_1 > \lambda_2 > \cdots > \lambda_k$ are distinct eigenvalues of $A(\Gamma)$ and their multiplicities are $m_1, m_2, \ldots, m_k$, respectively, then we shall write $Spec(\Gamma) = \left\{\lambda_1^{[m_1]}, \lambda_2^{[m_2]}, \ldots, \lambda_k^{[m_k]}\right\}$.

Let G be a non-trivial group, $S \subseteq G\{1\}$ and $S = S^{-1} := \{s^{-1} | s \in S\}$. The *Cayley graph* of G with respect to S, $Cay(G, S)$, is a graph with vertex set G, where two vertices a and b are adjacent if $ab^{-1} \in S$. The concept of Cayley graphs was introduced by Cayley [3]. Recently, the spectrum of some well-known chemical graphs are computed. For example, DeVos et al. [5] determined the spectrum of (3,6)−fullerenes, which are cubic plane graphs whose faces have sizes 3 and 6, for more details see [5]. They showed that every (3,6)−fullerene can be represented as a quotient of a certain lattice-like graph in the plane. Using this geometric description, they proved that these graphs are Cayley sum graphs and used a theorem which describes the spectral behavior of Cayley sum graphs in terms of group characters. In the same time, John and Sachs calculated the spectrum of toroidal graphs [15]. An n-fold periodic locally finite graph in the Euclidean n-space may be considered as the parent of an infinite class of n-dimensional toroidal finite graphs. In [15], an elementary method is developed that allows the characteristic polynomial of these graphs to be factored, in a uniform manner, into smaller polynomials, all of the same size. Applied to the hexagonal tessellation of the plane (the graphite sheet), this method enables the spectrum for all toroidal fullerenes and (3,6)−cages to be explicitly calculated. Also Alspach and Dean proved that honeycomb toroidal graphs, and hexagonal embeddings on a torus, are Cayley graphs on generalized dihedral groups [2]. Similar to [5], in this paper, we compute the spectrum of rhomboidal $C_4C_8(R)$ tori. Basic properties of graph eigenvalues and their applications in chemistry can be found in the famous book of Cvetković et al. [4].

Afshari and Maghasedi [1], by a theorem of Sabidussi [19], proved the following.

Theorem 1 (Afshari and Maghasedi [1]) *Let* $\Gamma = TUC_4C_8(R)[n, n]$. *Then* Γ *is a Cayley graph on* $G = \langle g_1, g_2, g_3, g_4 \rangle$ *with respect to* $S = \{g_3, g_1^{-1}g_2g_3g_4, g_1^{-1}g_4\}$, *where* $g_k: V(\Gamma) \to V(\Gamma)$, *1≤k≤4, are the maps* $g_1: v_{j,i}^t \to v_{j,(i-1)}^t$, $t = 0,1,2,3$; $g_2: v_{j,i}^t \to v_{(j+1),i}^t$, $t = 0,1,2,3$; $g_3: v_{j,i}^3 \to v_{i,j}^2$,

$v_{j,i}^2 \to v_{i,j}^2$, $v_{j,i}^1 \to v_{i,j}^0 \to v_{i,j}^1$; $g_4: v_{j,i}^3 \to v_{n-j+1,n-i+1}^0$, $v_{j,i}^2 \to v_{n-j+1,n-i+1}^1$, $v_{j,i}^1 \to v_{n-j+1,n-i+1}^2$, $v_{i,j}^0 \to v_{n-j+1,n-i+1}^0$ *and* $G = H \rtimes K$ *where* $H =< g_1, g_2 > \cong C_n \times C_n$ *is abelian and* $K =< g_3, g_4 > \cong C_2 \times C_2$.

In this paper, we determine the adjacency spectrum of $\Gamma = TRC_4C_8(R)[n,n]$. We also give lower and upper bounds for a chemical quantity, namely Estrada index, for a C_4C_8 net. The following is useful. Our approach is by using Irreducible representations of cyclic groups, direct product and some semidirect product groups.

Theorem 2 (Diaconis and Shahshahani [6]) *Consider the Cayley graph* $\Gamma = Cay(G,S)$. *Let* $Irr(G) = \{\rho_1, \dots, \rho_k\}$ *be the set of all non-equivalent irreducible representations of the group* G *and* d_i *denote the degree of* ρ_i *for* $i = 1,2 \dots, k$. *Let* ξ_i *denote the set of eigenvalues of* $\rho_i(S) := \sum_{s\in S} \rho_i(S)$ *for* $i = 1,2 \dots, k$. *Then, the set of all eigenvalues of adjacency matrix of* Γ *is equal to* $\cup_{i=1}^k \xi_i$. *Moreover, if the eigenvalue* λ *occurs with multiplicity* $m_i(\lambda)$ *in* $\rho_i(S)$, *then the multiplicity of* λ *in the adjacency spectrum is* $\sum_{i=1}^k d_i m_i(\lambda)$.

For more details and proofs regarding the previous theorem we refer to [6] and [16].

2. IRREDUCIBLE REPRESENTATIONS OF GROUPS

Irreducible representations of cyclic groups, direct products and some semi-direct product of groups are well known. Here, we present a few brief comments. Let us recall some facts from representation theory of groups, for more details see [17] and [20]. Let G be a cyclic group of order n generated by an element g . Then G has n *one* dimensional irreducible representations ρ_{ω^i}, $0 \le j \le n-1$, where $\rho_{\omega^i}(g^k) = \omega^{jk}$, $0 \le k \le n-1$ and $\rho = \exp\left(\frac{2\pi i}{n}\right)$. Let $W = G \times H$ be the direct product of two groups G and H. Thus the elements of W are the pairs (g,h), where $g \in G, h \in H$ and the multiplication in W is defined as $(g,h)(g',h') = (gg',hh')$. Let φ_G and Ψ_H be representations of G and H, respectively. Then for every $(g,h) \in W$, the Kronecker product $\theta(g,h) = \varphi_G(g) \otimes \Psi_H(h)$ is a representation of W. Furthermore, θ is an irreducible representation of W if and only if both of φ_G and Ψ_H are irreducible.

Now let us recall the induced representations. Let G be a finite group, and let H be a subgroup of index $n = |G:H|$. Suppose that φ_H is a representation of H of degree k and $G = Ht_1 \cup Ht_2 \cup \dots \cup Ht_n$ is a decomposition of G into right cosets of H, that is $t_1, t_2, \dots t_n$ is a right transversal of H in G. For every element x of G

we define a matrix $A(x)$ of degree kn as an $n \times n$ array of blocks, each of degree k, as follows:

$$A(x) = \begin{bmatrix} \widehat{\Phi}_H(t_1 x t_1^{-1}) & \cdots & \widehat{\Phi}_H(t_1 x t_n^{-1}) \\ \vdots & \ddots & \vdots \\ \widehat{\Phi}_H(t_n x t_1^{-1}) & \cdots & \widehat{\Phi}_H(t_n x t_n^{-1}) \end{bmatrix} \tag{2.1}$$

where $\widehat{\Phi}_H(g) = \widehat{\Phi}_H(g)$ if $g \in H$ and 0 otherwise. Indeed A is a representation of G. In the construction of $A(x)$, we employed a particular transversal, but this choice does not materially affect the result, for more details see [17,69–71].

Let $G = HK$ be a semi-direct product of groups with abelian normal subgroup H. Since H is abelian, its irreducible characters are of degree 1 and they form a group X. The group G acts on X by $\chi^g(h) \coloneqq \chi(ghg^{-1})$, where $g \in G$, $\chi \in X$ and $h \in H$. Let $\chi_i^k = \{\chi_i^k |\, k \in K\}$, $1 \leq i \leq r$ and r is the number of conjugacy classes of H, be orbits of the action of K on X with representatives χ_i, respectively. For $1 \leq i \leq r$, let $K_i = k_{\chi_i} = \{k \in K \,|\chi_i^k = \chi_i\}$ be the stabilizer of χ_i in K and $G_i = HK_i$ be the corresponding subgroup of G. Extend χ_i to G_i by setting $\hat{\chi}_i(hk) = \chi_i(h)$ for $h \in H$ and $k \in K_i$. Using the fact that $\chi_i^k = \chi_i$, we see that $\hat{\chi}_i$ is a character of degree 1 of G_i. Now let ρ be an irreducible representation of K_i. By composing ρ with the canonical projection $\pi: G_i \to K_i$ we obtain an irreducible representation $\tilde{\rho} = \rho o \pi$ of G_i. Finally, by taking the tensor product of $\hat{\chi}_i$ and $\tilde{\rho}$, we will obtain an irreducible representation $\hat{\chi}_i \otimes \tilde{\rho}$ of G_i. Let $\theta_{i,p} = \hat{\chi}_i \otimes \tilde{\rho} \uparrow G$ be the corresponding induced representation of G. Then the set of all irreducible non-equivalent representations of G is

$$Irr(G) = \{\theta_{i,p} | 1 \leq i \leq r, \rho \in Irr(K_i)\}.$$

The interested readers can consult [20, 62–63] for more information on this algorithm. Let L be a subgroup of G and for each representation $f: L \to GL_k(\mathbb{C})$

$$\hat{f}(x) = \begin{cases} f(x) & x \in L \\ 0 & otherwise \end{cases}.$$

3. MAIN RESULTS

We first give the irreducible representation of the group $G = < g_1, g_2, g_3, g_4 >$ as defined in Theorem 1. Let $\omega = \exp\left(\frac{2\pi i}{n}\right)$, R_1 be the set of all representatives of orbits of the action of K on $Irr(H)$ (as defined above) with length four when n is even and R_2 be the set of all representatives of orbits of the action of K on $Irr(H)$ with length four when n is odd. Let $Y_1 = \{1, 2, \dots, \frac{n}{2} - 1\}$ and $Y_2 = \{1, 2, \dots, \frac{n-1}{2}\}$. Consider $x = g_1^l g_2^m g_3^u g_4^v \in G$ as an arbitrary element of G. We define below maps:

$$\zeta_{p,q}: x \to (-1)^{pu+qv} \qquad 0 \leq p, q \leq 1,$$

$$\eta_{p,q}: x \to (-1)^{1+m+pu+qv} \quad 0 \le p,q \le 1,$$
$$\theta_p: x \to \begin{bmatrix} \hat{f}(x) & \hat{f}(xg_3) \\ \hat{f}(g_3x) & \hat{f}(g_3xg_3) \end{bmatrix} \quad 0 \le p \le 1$$
$$\vartheta_{p,r}: x \to \begin{bmatrix} \hat{g}(x) & \hat{g}(xg_4) \\ \hat{g}(g_4x) & \hat{g}(g_4xg_4) \end{bmatrix} \quad 0 \le p \le 1, r \in Y_1$$
$$\iota_{p,r}: x \to \begin{bmatrix} \hat{h}(x) & \hat{h}(xg_3) \\ \hat{h}(g_3x) & \hat{h}(g_3xg_3) \end{bmatrix} \quad 0 \le p \le 1, r \in Y_1$$
$$\kappa_{r,s}: x \to \begin{bmatrix} \hat{\imath}(x) & \hat{\imath}(xg_3) & \hat{\imath}(xg_4) & \hat{\imath}(xg_3g_4) \\ \hat{\imath}(g_3x) & \hat{\imath}(g_3xg_3) & \hat{\imath}(g_3xg_4) & \hat{\imath}(g_3xg_3g_4) \\ \hat{\imath}(g_4x) & \hat{\imath}(g_4xg_3) & \hat{\imath}(g_4xg_4) & \hat{\imath}(g_4xg_3g_4) \\ \hat{\imath}(g_3g_4x) & \hat{\imath}(g_3g_4xg_3) & \hat{\imath}(g_3g_4xg_4) & \hat{\imath}(g_3g_4xg_3g_4) \end{bmatrix}, (r,s) \in R_1$$

where f, g, h, i are linear representations of $H < g_4 >, H < g_3 >, H < g_3g_4 >$ and H, respectively, with $f(g_1^l g_2^m g_4^v) = (-1)^{m+pu}$, $g(g_1^l g_2^m g_4^u) = h(g_1^l g_2^m (g_3g_4)^u)\omega^{r(1-m)}(-1)^{pu} = \omega^{r(1+m)}(-1)^{pu}$, and $i(g_1^l g_2^m) = \omega^{rl+sm}$. We keep these notations after this.

Lemma 1. *Let* $G =< g_1, g_2, g_3, g_4 >$ *be the group defined in Theorem 1. If* n *is even, then*

$$Irr(G) = \{\zeta_{p,q}, \eta_{p,q}, \theta_p, \vartheta_{p,q}, \iota_{p,r}, \kappa_{r',s} \mid 0 \le p,q \le 1, r \in Y_1, (r',s) \in R_1\},$$

and if n *is odd, then*

$$Irr(G) = \{\zeta_{p,q}, \vartheta_{p,q}, \iota_{p,r}, \kappa_{r',s} \mid 0 \le p,q \le 1, r \in Y_2, (r',s) \in R_2\}.$$

Proof. By Theorem 1, $G = H \rtimes K$, where $H =< g_1, g_2 >\cong C_n \times C_n$ is abelian and $K =< g_3, g_4 >\cong C_2 \times C_2$. Let

$$X \coloneqq \{Irr(G) = \{\chi_{r,s} \mid \chi_{r,s}(g_1^l g_2^m) = \omega^{rl+sm}, 0 \le r,s,l,m \le n-1\}.$$

We now consider the action of G on X as defined before. Using the relations between the generators of the group G, which are given in the proof of Theorem 1, one can easily check that the restriction of this action to the subgroup K is given by $\chi_{r,s}^1 = \chi_{r,s}, \chi_{r,s}^{g_3} = \chi_{n-s,n-r}, \chi_{r,s}^{g_4} = \chi_{n-r,n-s}, \chi_{r,s}^{g_3g_4} = \chi_{s,r}$.

Let $\bar{n} = \{0,1,\dots,n-1\}$, $A = \{(n_1,n_2) | n_1,n_2 \in \bar{n}\}$ and

$T_1 = A - \{(0,0), (\frac{n}{2},\frac{n}{2}), (0,\frac{n}{2}), (\frac{n}{2},0), (r,n-r), (n-r,r), (r,r), (n-r,n-r) | r \in Y_1\}$,

$T_2 = A - \{(0,0), (r,n-r), (n-r,r), (r,r), (n-r,n-r) | r \in Y_2\}$.

Note that the length of an orbit with representative $\chi_{r,s}$ is four if and only if $(r,s) \in T_1$ when n is even and $(r,s) \in T_2$ when n is odd. The partition of X into its orbits is given in Tables 1 and 2 when n is even and odd, respectively. If we choose a representative of each orbit of X, as given in Table 1, when n is even, then we have the corresponding stabilizers as follows.

Table 1: K–orbits of $Irr(H)$ when n is even.

Representative	Elements
$\chi_{0,0}$	$\chi_{0,0}$
$\chi_{\frac{n}{2},\frac{n}{2}}$	$\chi_{\frac{n}{2},\frac{n}{2}}$
$\chi_{0,\frac{n}{2}}$	$\chi_{0,\frac{n}{2}}, \chi_{\frac{n}{2},0}$
$\chi_{r,n-r}, r \in Y_1$	$\chi_{r,n-r}, \chi_{n-r,r}$
$\chi_{r,r}, r \in Y_1$	$\chi_{r,r}, \chi_{n-r,n-r}$
$\chi_{r,s}, (r,s) \in T_1$	$\chi_{r,s}, \chi_{s,r}, \chi_{n-r,n-s}, \chi_{n-s,n-r}$

$K_{0,0} = K_{\frac{n}{2},\frac{n}{2}} = K$, $K_{0,\frac{n}{2}} =< g_4 >$, $K_{1,n-1} = K_{2,n-2} = \cdots = K_{\frac{n}{2}-1,\frac{n}{2}+1} =< g_3 >$, $K_{1,1} = K_{2,2} = \cdots = K_{\frac{n}{2}-1,\frac{n}{2}-1} =< g_3 g_4 >$ and $k_{r,s} = 1$, when $(r,s) \in T_1$. Note that the length of R_1 is $\frac{n(n-2)}{4}$. Also when n is odd, $K_{0,0} = K$, $K_{1,n-1} = K_{2,n-2} = \cdots = K_{\frac{n-1}{2},\frac{n+1}{2}} =< g_3 >$ and $K_{1,1} = K_{2,2} = \cdots = K_{\frac{n-1}{2},\frac{n+1}{2}} =< g_3 g_4 >$ and $k_{r,s} = 1$, when $(r,s) \in T_2$. Note that the length of R_2 is $\frac{(n-2)^2}{4}$.

On the other hand, $Irr(G) = \{\rho_{p,q} | \rho_{p,q}(g_3^u g_4^v) = (-1)^{pu+pv}, 0 \leq p,q,u,v \leq 1\}$ and when $g \in \{g_3, g_4, g_3 g_4\}$, $Irr(< g >) = \{\rho_p | \rho_p(g^u) = (-1)^{pu}, 0 \leq p,u \leq 1\}$. Now it is enough to follow the procedure of computing the irreducible representations of a semi-direct product group with an abelian normal subgroup as we recalled before. □

Table 2: k–orbits of $Irr(H)$ when n is odd.

Representative	Elements
$\chi_{0,0}$	$\chi_{0,0}$
$\chi_{r,n-r}, r \in Y_2$	$\chi_{r,n-r}, \chi_{n-r,r}$
$\chi_{r,r}, r \in Y_2$	$\chi_{r,r}, \chi_{n-r,n-r}$
$\chi_{r,s}, (r,s) \in T_2$	$\chi_{r,s}, \chi_{s,r}, \chi_{n-r,n-s}, \chi_{n-s,n-r}$

By Theorems 1 and 2 and Lemma 1, we have the following.

Theorem 3 *Let* $\Gamma = TRC_4C_8(R)[n,n]$ *and* $\alpha_r = \cos(\frac{2\pi r}{n})$ *for all* r. *If* n *is even, then* $Spec(\Gamma) = \left\{\pm 3, (\pm 1)^{[5]}, (\pm\sqrt{5})^{[2]}\right\} \cup \cup_{r \in Y_1} \left\{\left(\pm_a 1 \pm_b \sqrt{2 \pm_a 2\alpha_r}\right)^{[4]}\right\}$ $\cup \cup_{(r',s) \in T_1} \{\lambda^{[4]} | \lambda^4 - 6\lambda^2 - 4\lambda(\alpha_{r'} + \alpha_s) + 1 - 4\alpha_{r'}\alpha_s = 0\}$ *and if* n *is odd, then we have* $Spec(\Gamma) = \{3, (\pm 1)^{[3]}\} \cup \cup_{r \in Y_2} \left\{\left(\pm_a 1 \pm_b \sqrt{2 \pm_a 2\alpha_r}\right)^{[4]}\right\}$ $\cup$

$\cup_{(r',s)\in T_2}\{\lambda^{[4]}\,|\lambda^4-6\lambda^2-4\lambda(\alpha_{r'}+\alpha_s)+1-4\alpha_{r'}\alpha_s=0\}$, *where two symbols* $\pm_a$ *have the same sign, while the sign of* $\pm_b$ *is independent.*

Proof. By Theorem 1, we know that $\Gamma = Cay(G,S)$, where $G =< g_1, g_2, g_3, g_4 > \cong (C_n \times C_n) \rtimes (C_2 \times C_2)$ and $S = \{g_3, g_1^{-1}, g_2g_3g_4, g_1^{-1}g_4\}$. We consider the following two cases.

Case 1. n is even. By Lemma 1, we have

$$Irr(G) = \{\zeta_{p,q}, \eta_{p,q}, \theta_p, \vartheta_{p,q}, \iota_{p,r}, \kappa_{r',s} | 0 \le p,q \le 1, r \in Y_1, (r',s) \in R_1\}.$$

Using the relations between the generators of G given in the proof of Theorem 1, one can easily see that $\zeta_{p,q}(S) = \sum_{s\in S}\zeta_{p,q}(S) = (-1)^p + (-1)^{p+q} + (-1)^q$, $\eta_{p,q}(S) = (-1)^p + (-1)^{p+q} + (-1)^{q-1}$,

$$\theta_p(S) = \begin{bmatrix} (-1)^p & 1-(-1)^p \\ 1-(-1)^p & (-1)^{p+1} \end{bmatrix},$$

$$\vartheta_{p,q}(S) = \begin{bmatrix} (-1)^p & \omega^{-r}+(-1)^p \\ \omega^{-r}+(-1)^p & (-1)^p \end{bmatrix},$$

$$\iota_{p,r}(S) = \begin{bmatrix} (-1)^p & 1+\omega^{-r}(-1)^p \\ 1+\omega^{-r}(-1)^p & (-1)^p \end{bmatrix},$$

$$\kappa_{r',s} = \begin{bmatrix} 0 & 1 & \omega^{-r'} & \omega^{-r'+s} \\ 1 & 0 & \omega^{-r'+s} & \omega^{s} \\ \omega^{r'} & \omega^{r'-s} & 0 & 1 \\ \omega^{r'-s} & \omega^{-s} & 1 & 0 \end{bmatrix}.$$

So, we have:

$$Spec(\zeta_{p,q}(S)) = \{(-1)^p + (-1)^{p+q} + (-1)^q\},$$

$$Spec(\eta_{p,q}(S)) = \{(-1)^p + (-1)^{p+q} + (-1)^{q-1}\},$$

$$Spec(\theta_1(S)) = \{\pm\sqrt{5}\}, Spec(\theta_0(S)) = \{\pm 1\},$$

$$Spec\left(\vartheta_{0,r}(S)\right) = Spec\left(\iota_{0,r}(S)\right) = \{1 \pm \sqrt{2+2\alpha_r}\},$$

$$Spec\left(\vartheta_{1,r}(S)\right) = Spec\left(\iota_{1,r}(S)\right) = \{-1 \pm \sqrt{2-2\alpha_r}\},$$

$$Spec\left(\kappa_{r',s}(S)\right) = \{\lambda^4 - 6\lambda^2 - 4\lambda(\alpha_{r'}+\alpha_s) + 1 - 4\alpha_{r'}\alpha_s = 0\}.$$

Note that $\kappa_{r',s}(S)$ is a Hermitian matrix and so its eigenvalues are real. Since the degrees of the representations $\zeta_{p,q}$, $\eta_{p,q}$, θ_p, $\vartheta_{p,r}$, $\iota_{p,r}$ and $\kappa_{r',s}(S)$ are 1, 1, 2, 2, 2 and 4, respectively, the result follows by Theorem 2.

Case 2. n is odd. By Lemma 1,

$$Irr(G) = \{\zeta_{p,q}, \vartheta_{p,r}, \iota_{p,r}, \kappa_{r',s} | 0 \le p,q \le 1, r \in Y_2, (r',s) \in T_2\}.$$

By a similar argument, one can easily obtain the result. □

Note that $(r',s) \in T$, then $\chi^k_{r',s} = \{\chi_{r',s}, \chi_{s,r'}, \chi_{n-r',n-s}, \chi_{n-s,n-r'}\}$. Let $f_{r',s}(\lambda) := \lambda^4 - 6\lambda^2 - 4\lambda(\alpha_{r'} + \alpha_s) + 1 - 4\alpha_{r'}\alpha_s$. It is clear that $f_{s,r'}(\lambda) = f_{r',s}(\lambda)$, $\alpha_{n-r'} = \alpha_{r'}$and $\alpha_{n-s} = \alpha_s$. So $f_{r',s} = f_{s,r'} = f_{n-r',n-s} = f_{n-s,n-r'}$. Therefore we can arbitrarily choose any element of an orbit of length four as representative. This shows that our calculations are true.

Let us give the following examples to clear our procedure.

Example 1 *If* $n = 3$ then $Y_2 = \{1\}$, $T_2 = \{(0,1),(1,0),(0,2),(2,0)\}$ *and* $R_2 = \{(0,1)\}$. *Therefore, by Corollary 3,*

$$Spec_A(\Gamma) = \{3, (-1)^{[7]}, \left(-1 \pm \sqrt{3}\right)^{[4]}, 0^{[4]}, 2^{[4]}, \alpha^{[4]}, \beta^{[4]}, \gamma^{[4]}\},$$

where α, β *and* γ *are the roots of* $x^3 - x^2 - 5x + 3 = 0$. *Note that* $\alpha \approx 2.51414$, $\beta \approx -2.08613$ *and* $\gamma \approx 0.571993$.

Example 2 *If* $n = 4$ *then we have* $Y_1 = \{1\}$, $T_1 = \{(0,1),(1,0),(0,3),(3,0),(1,2),(2,1),(3,2),(2,3)\}$ *and* $R_1 = \{(0,1),(1,2)\}$. *So by Theorem 3,*

$$Spec_A(\Gamma) = \{\pm 3, (\pm 1)^{[9]}, \left(\pm\sqrt{5}\right)^{[2]}, \left(1 \pm \sqrt{2}\right)^{[4]}, \left(-1 \pm \sqrt{2}\right)^{[4]}, (\pm\alpha)^{[4]}, (\pm\beta)^{[4]}, (\pm\gamma)^{[4]}\},$$

where α, β *and* γ *are roots of* $x^3 - x^2 - 5x + 1 = 0$. *An easy calculation shows that* $\alpha \approx 2.70928$, $\beta \approx -1.90321$ *and* , $\gamma \approx 0.193937$.

At the end of this paper, using Theorem 3, we give lower and upper bounds for an important chemical quantity, namely Estrada index, for the graph. The Estrada index $EE(\Gamma)$ of the graph Γ is defined as the sum of the terms e^λ , $\lambda \in Spec(\Gamma)$. This quantity, which introduced by Ernesto Estrada, has noteworthy chemical applications, see [4, 10, 11, 13, 14, 18] for details. Using Theorem 3, we can obtain the following.

Corollary 1 *Let* $\Gamma = TRC_4C_8[n,n]$,$\beta = e\cosh\sqrt{2 + 2\alpha_r} + e^{-1}\cosh\sqrt{2 - 2\alpha_r}$ *and* $\alpha_r = \cos(\frac{2\pi r}{n})$. *If* $n \neq 2$ *is even, then*

$$1 \leq \frac{EE(\Gamma) - 2(\cosh 3 + 5\cosh 1 + 2\cosh\sqrt{5} + 4\sum_{r=1}^{\frac{n}{2}-1}\beta_r)}{4(n^2 - 2n)} < e^3$$

and if $n \neq 1$ *is odd, then* $1 \leq \frac{EE(\Gamma) - e^3 - 3e^{-1} - 8\sum_{r=1}^{\frac{n}{2}-1}\beta_r}{4(n^2 - 2n)} < e^3$.

Proof. We have $EE(\Gamma) = \sum_{\lambda\in Spec(\Gamma)} e^{\lambda}$. By Theorom 3, we know that when n is even, $Spec(\Gamma) = \{\pm 3, (\pm 1)^{[5]}, (\pm\sqrt{5})^{[2]}\} \cup \cup_{r\in Y_1} \left\{\left(\pm_a 1 \pm_b \sqrt{2\pm_a 2\alpha_r}\right)^{[4]}\right\}$ $\cup\cup_{(r',s)\in R_1} \{\lambda^{[4]} \,|\lambda^4 - 6\lambda^2 - 4\lambda(\alpha_{r'} + \alpha_s) + 1 - 4\alpha_{r'}\alpha_s = 0\}$. Let $f_{r',s}(\lambda) = \lambda^4 - 6\lambda^2 - 4\lambda(\alpha_{r'} + \alpha_s) + 1 - 4\alpha_{r'}\alpha_s$, $(r', s) \in T_1$, and $\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4$ be the roots of $f_{r',s}$. From inequality of arithmetic and geometric means, we have

$$\sqrt[4]{e^{\sum_{i=1}^{4}\lambda_i}} \le \frac{\sum_{i=1}^{4} e^{\lambda_i}}{4} \le e^{\lambda_1} \tag{3.2}$$

Since the coefficient of λ^3 in $f_{r',s}(\lambda)$ is 0, we have $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 0$. On the other hand Γ is a 3-regular graph and so by Perron-Frobenius theorem, $\lambda_1 < 3$ (See [12, p.178].). Therefore by (3.2),

$$4 \sum_{i=1}^{4} e^{\lambda_i} < 4e^3 \tag{3.3}$$

We know that for every real number x, $e^x + e^{-x} = 2\cosh x$. Thus when n is even, we have

$$EE(\Gamma) = 2(\cosh 3 + 5\cosh 1 + 2\cosh\sqrt{5} + 4e\sum_{r=1}^{\frac{n}{2}-1} \cosh\sqrt{2 + 2\alpha_r} + 4e^{-1}\sum_{r=1}^{\frac{n}{2}-1} \cosh\sqrt{2 - 2\alpha_r} + 4\sum_{(r',s)\in T_1} \sum_{\lambda_i f_{r',s}=0} e^{\lambda}).$$

By inequality (3.3), $4 \le \sum_{\lambda_i f_{r',s}=0} e^{\lambda} < 4e^3$. Also as we saw in the proof of Lemma 1, the length of T_1 is $\frac{n^2-2n}{4}$ and therefore, $1 \le \frac{4\sum_{(r',s)\in R_1}\sum_{\lambda_i f_{r',s}=0} e^{\lambda}}{4(n^2-2n)} < e^3$. This completes the proof of corollary in this case. Assume now that n is odd. From Theorem 3, $Spec(\Gamma) = \{3, (\pm 1)^{[3]}\} \cup\cup_{r\in Y_2} \left\{\left(\pm_a 1 \pm_b \sqrt{2\pm_a 2\alpha_r}\right)^{[4]}\right\}$ $\cup\cup_{(r',s)\in T_2} \{\lambda^{[4]} \,|\lambda^4 - 6\lambda^2 - 4\lambda(\alpha_{r'} + \alpha_s) + 1 - 4\alpha_{r'}\alpha_s = 0\}$. By the fact that the length of T_2 is $\frac{(n-1)^2}{4}$ and inequality (3.3), one can similarly get the result. □

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