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Topological Indices of Certain Graphs

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ABSTRACT

In this paper we first consider and study certain edge-transitive connected graphs, such as the Hamming graphs, the Paley graphs and the Boolean lattice. Then as a consequence, we obtain the Wiener and the hyper-Wiener indices of these graphs.

1. INTRODUCTION

In what follows $G = (V, E)$ is a connected simple graph with vertex set V and edge set E. The Wiener index which is introduced by H. Wiener in [10], is the first topological index used in chemistry and it has an important role in the molecular graph theory. This index is equal to the sum of distances between all pairs of vertices of a graph, i.e. $W(G) = \sum_{\{u,v\}\subseteq V} d(u, v)$. In 1993 the hyper-Wiener index was introduced by Milan Randic for

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acyclic graphs. Later, in 1995, Randić's definition was generalized by Klein et al. in [6] for all connected graphs. This generalization is called hyper-Wiener index of G and it is defined as $WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V} d^2(u,v)$, where $d(u,v)$ is the distance between vertices u and v. We refer the reader to [2] for more detailed information on these two indices and also for their mathematical properties and applications in chemistry. In this article we compute the Wiener and hyper-Wiener index of a special class of graphs where the first ones are called Hamming graphs (named after Richard Hamming). These graphs are used in several branches of mathematics, also in chemistry and computer science.

Let S be a set of q elements and d a positive integer. The Hamming graph $H(d,q)$ has vertex set S^d, which is the set of ordered d-tuples of elements in S. Two vertices u and v in $H(d,q)$ are adjacent if they differ in exactly one entry.

The Hamming graph $H(d,q)$, which is briefly observed that is isomorphic to the Cartesian product of d complete graphs K_q, it is also $d(q-1)$-regular graph. By considering the formula, $\sum_{v\in} \delta(v) = 2|E|$, where $\delta(v)$ is the degree of the vertex v and $|E|$ is the number of edges in the graph, there are $\frac{1}{2}d(q-1)q^2$ edges in the Hamming graph $H(d,q)$. Moreover, the diameter of $H(d,q)$ is d, as the maximum distance occurs when the two vertices differ in all d co-ordinates.

2. AUTOMORPHISM GROUP OF $H(d,q)$

An automorphism of the graph $T = (V,E)$ is a permutation of V, which maps adjacent vertices to adjacent vertices and non-adjacent vertices to non-adjacent vertices. The set of all the automorphisms of T is denoted by $Aut(T)$ which is a permutation group. In the following two propositions, of which the first one is well-known, we will observe that $Aut(H(d,q))$ has a subgroup that is regular on vertices. Consequently, by [9], we infer that Hamming graphs are Cayley graphs too.

We first recall the following well-known definitions.

Definition 2.1. Let A be a group and let H be a group acting on a set Ω (on the left). The direct product A^Ω of A with itself indexed by Ω is the set of sequences $\bar{a} = (a_\omega)_{\omega\epsilon\Omega}$ in A indexed by Ω, with a group operation given by pointwise multiplication. The action of H on Ω can be extended to an action on A^Ω by reindexing, namely by defining $h.(a_\omega)_{\omega\epsilon\Omega} := (a_{h^{-1}\omega})_{\omega\epsilon\Omega}$, for all $h \in H$ and all $(a_\omega)_{\omega\epsilon\Omega} \in A^\Omega$. Then the wreath product $A \wr H$ of A by H is the semidirect product $A^\Omega \rtimes H$ with the action of H on A^Ω given above.

Definition 2.2. Let G be a group and S a nonempty subset of G not containing the identity and $S = S^{-1}$. The Caley graph of G with respect to S, written $Cay(G,S)$ is a graph with vertex set G and edge set $E = \{ (a,b) |\, a,b \in G, a^{-1}b \in S \}$.

Proposition 2.3. $Aut(H(d,q)) = \mathbb{S}_d \wr \mathbb{S}_q$.

Proof. See [7]. ∎

Proposition 2.4. $Aut(H(d,q))$ *has a subgroup that is regular on vertices.*

Proof. For $\sigma \in \mathbb{S}_d$, define

$$(x_1, \dots, x_d)^\sigma \coloneqq (x_{(1)\sigma}, \dots, x_{(d)\sigma}),$$

then $\boldsymbol{\sigma}$ is an automorphism of the Hamming graph $H(d,q)$ and therefore $\mathbb{S}_{\boldsymbol{d}} \leq Aut(H(d,q))$. ∎

Corollary 2.5. $H(d,q)$ *is a Cayley graph.*

Proof. By Proposition 2.4 and [9] we are done. ∎

In view of the following definition it is clear as we mentioned earlier that $H(d,q)$ is a product of d-copies of the complete graph K_q.

Definition 2.6. Let G and H be graphs. The Cartesian product $G \times H$ is the graph with vertices the Cartesian product $V(G) \times V(H)$ and two vertices (u,u') and (v,v') are adjacent if and only if either $u = v$ and u' is adjacent to v' in H or $u' = v'$ and u is adjacent to v in G.

As the Hamming graph $H(d,q)$ is the d-fold Cartesian product of K_q, one may describe it as a Cayley graph $Cay(G,\Delta)$,

$$G = \underbrace{F \times \dots \times F}_{d-times} = F^d$$

with F the additive group of the field F, $|F| = q$ and $\Delta = \{(0,0,\dots,0,a,0,\dots,0) | 0 \neq a \epsilon F\}$.

3. WIENER AND HYPER–WIENER INDEX OF $H(d,q)$

In this section we will compute the Wiener index and the hyper-Wiener index of $H(d,q)$ by considering $H(d,q)$ as a Cartesian product of d-fold complete graph K_q and using the Wiener and hyper-Wiener formulas for the Cartesian product of graphs in [5]. Before finding these indices, as an example, we first draw the reader's attention to the following computed hyper-Wiener index of the one-pentagonal carbon nanocone. The graph of this molecule consists of one pentagone surrounded by layers of hexagons. If there are *n* layers, then this graph is denoted by G_n.

Example 3.1. [2] The hyper-Wiener index of the graph of one-pentagonal carbon nanocone G_n is,

$$WW\ (G_n) = 20 + \frac{533}{4}n + \frac{8501}{24}n^2 + \frac{5795}{12}\ n^3 + \frac{8575}{24}n^4 + \frac{409}{3}n^5 + 21n^6\ .$$

Proposition 3.2. *The Wiener index of $H(d,q)$ is equal to* $\frac{q^{2d}(q-1)d}{2q}$.

Proof. By [5], the Wiener index of the Cartesian graph $G \times H$ is as follows

$$W(G \times H) = |V(H)|^2 W(G) + |V(G)|^2 W(H),$$

and therefore, by an inductive argument we can see that $W(\otimes_{i=1}^{n} G_i) = |V|^2 \sum_{i=1}^{n} \frac{W(G_i)}{|V_i|^2}$, where $V = V(\otimes_{i=1}^{n} G_i)$. Since $H(d,q) = \otimes_d K_q$, and recalling the Wiener index formula for the connected simple graph [1], we infer that

$$W(K_q) = \frac{1}{2}\sum_{v \in V(K_q)} d(v),$$

Where $d(v) = \sum_{x \in V(K_q)} d(v,x) = q - 1$. Hence, $W(K_q) = \frac{1}{2}q(q-1)$. This implies that

$$W\big(H(d,q)\big) = W(\bigotimes_{d} K_q) = q^{2d} \sum_{i=1}^{d} \frac{q(q-1)}{2q^2} = \frac{q^{2d}(q-1)d}{2q}.$$

Proposition 3.3. *The hyper-Wiener index of $H(d,q)$ is equal to*

$$\frac{1}{4} dq^{2d-2}(q-1)\big(2q + (d-1)(q-1)\big).$$

Proof. By [5], for the Cartesian graph $G \times H$, the hyper-Wiener index of $G \times H$ which is denoted by $WW(G \times H)$, is as follows

$$WW(G \times H) = |V(H)|^2 WW(G) + |V(G)|^2 WW(H) + 2W(G)W(H).$$

By applying an induction argument and considering the formula of the hyper-Wiener index for Cartesian product of two graphs in [5], it is shown that,

$$WW(G^n) = n|V(G)|^{2n-4}\big(|V(G)|^2 WW(G) + (n-1)W^2(G)\big).$$

Therefore by applying the formula for K_q^d we have

$$WW(K_q^d) = dq^{2q-4}\left(q^2 WW(K_q) + (d-1)W^2(K_q)\right).$$

We also recall that for a graph G,

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\} \subseteq V(G)} d^2(u,v),$$

where $d^2(u,v) = d(u,v)^2$.

This implies that $WW(K_q) = \frac{1}{2}W(K_q) + \frac{1}{4}\sum_{v\in V(K_q)} d(v) = \frac{1}{4}q(q-1) + \frac{q(q-1)}{4} = \frac{q(q-1)}{2}$. Finally, we have

$$\begin{aligned} WW(H(d,q)) &= WW(K_q^d) \\ &= dq^{2d-4}\left(q^2\frac{q(q-1)}{2} + (d-1)\left(\frac{q(q-1)}{2}\right)^2\right) \\ &= \frac{1}{4}dq^{2d-2}(q-1)\big(2q+(d-1)(q-1)\big), \end{aligned}$$

which completes the proof. ∎

4. WIENER AND HYPER–WIENER INDICES OF THE PALEY GRAPH

Some topological indices of Paley graph was computed in [8], such as the Wiener index, the PI index and the Szeged index. In this section we compute the hyper-Wiener index of the Paley graph, but since the Wiener index of this graph is needed, we calculate it again in this section.

Without further ado let us start with the following definition.

Definition 4.1. Let F_q denote the field with q elements, where $q \equiv 1\ (mod\ 4)$. The Paley graph $P(q)$ has F_q as the set of its vertices and two vertices x and y are joined by an edge if and only if $x - y$ is a non-zero square in F_q.

We put $S = \{a^2 | 0 \neq a \in F_q\}$. Then clearly $P(q)$ is the Caley graph of the additive group of F_q with S as the connecting set. The condition $q \equiv 1\ (mod\ 4)$ implies that $-1 \in F_q$, hence $S = -S$ and $P(q)$ is an undirected graph. Because S generates F_q we deduce that $P(q)$ is a connected graph. $P(q)$ is a regular graph of degree $\frac{q-1}{2}$, hence the number of edges in $P(q)$ is $\frac{q(q-1)}{4}$.

For the automorphism group of $P(q)$ we refer the reader to [4]. By construction of $P(q)$ the graph $P(q)$ has the following automorphisms : translation by an element of F_q, multiplication by an element of S, and by applying any field automorphism of F. For q odd these operations generate the group

$$A\Delta L_1(q) = \{v \mapsto av^\gamma + b \,|\, a \in S, b \in F_q, \gamma \in Aut(F_q)\}.$$

Therefore $AutP(q)$ has a subgroup isomorphic to $A\Delta L_1(q)$. In fact by [4] we have:

Proposition 4.2. *If* $q \equiv 1\ (mod\ 4)$ *then* $AutP(q) \cong A\Delta L_1(q)$.

We see that $P(q)$ is of diameter 2 and its automorphism acts transitively on its vertices. In what follows V denotes the set of vertices of the graph.

Theorem 4.3. [8] *The Wiener index of* $P(q)$ *is* $\frac{3q(q-1)}{4}$.

Proof. Because of vertex-transitivity of $P(q)$, by [1] we have $W\big(P(q)\big)=\frac{1}{2}|V|d(v)=\frac{q}{2}d(v)$, where $d(v)=\sum_{x\in V}d(v,x)$, for v a fixed vertex of $P(q)$. Let $v=0$, then $d(v)=\sum_{x\in V}d(0,x)$. If x is a square, then $d(0,x)=1$, otherwise $d(0,x)=2$. Therefore $d(v)=\frac{q-1}{2}+2\frac{(q-1)}{2}=\frac{3(q-1)}{2}$. Thus $W\big(P(q)\big)=\frac{3q(q-1)}{4}$. ■

Theorem 4.4. *The hyper-Wiener index of* $P(q)$ *is* $q(q-1)$.

Proof. By definition we have $WW(P(q)=\frac{1}{2}W\big(P(q)\big)+\frac{1}{2}\sum_{\{u,v\}\subseteq V}d(u,v)^2$. Now by invoking again [1] and putting $D(v)=\sum_{x\in V}d(v,x)^2$, we get $WW(G)=\frac{1}{4}|V|d(v)+\frac{1}{4}|V|D(v)$. But $D(v)=\sum_{x\in V}d(v,x)^2=\frac{q-1}{2}+\frac{4(q-1)}{2}=\frac{5(q-1)}{2}$, therefore $WW\big(P(q)\big)=\frac{3q(q-1)}{8}+\frac{5q(q-1)}{8}=q(q-1)$. ■

5. THE WIENER AND HYPER–WIENER INDEX OF THE BOOLEAN LATTICE

In the following we define the Boolean lattice.

Definition 5.1. The Boolean lattice $BL_n, n\geq 1$, is the graph whose vertex set is the set of all subsets of $\{1,2,\dots,n\}$ where two subsets x and y are joined by an edge if their symmetric difference $x\cup y\backslash x\cap y$ has size 1.

The hypocube Q_n is a graph whose vertices are elements of $\{0,1\}^n$ and two vertices are joined by an edge if they differ in only one place. It is not difficult to show that $BL_n\cong Q_n$. By [1] the automorphism group of Q_n is isomorphic to the group $2^n\rtimes\mathbb{S}_n$, where $2^n$is the elementary abelian group of order 2^n. In [1] it is also proved that $Aut(Q_n)$ acts transitively on the set of vertices of Q_n, and it is computed as $W(Q_n)=2^{2(n-1)}n$.Therefore here we compute the hyper-Wiener index of Q_n. Before finding this index, let us digress for a moment and prove the following Lemma for the sake of the reader.

Lemma 5.2.

$$\sum_{j=0}^{n}j\binom{n}{j}=n\times 2^{n-1},$$

$$\sum_{j=0}^{n}j^2\binom{n}{j}=(n+1)n\times 2^{n-2}.$$

Proof. Consider the identity $(x+1)^n=\sum_{j=0}^{n}\binom{n}{j}x^j$ and differentiate both sides with respect to x,

$$n(x+1)^{n-1} = \sum_{j=0}^{n} j \binom{n}{j} x^{j-1} \quad (1)$$

By substituting $x = 1$ we obtain $\sum_{j=0}^{n} j \binom{n}{j} = n \times 2^{n-1}$. Now if we differentiate both sides of (1) with respect to x we get,

$$n(n-1)(x+1)^{n-2} = \sum_{j=0}^{n} j(j-1) \binom{n}{j} x^{j-2}$$

If we substitute $x = 1$, we obtain $n(n-1)2^{n-2} = \sum_{j=0}^{n} (j^2 - j) \binom{n}{j}$ and finally

$$\sum_{j=0}^{n} j^2 \binom{n}{j} = (n+1)n \times 2^{n-2}.$$ ■

Theorem 5.3. *The hyper-Wiener index of* Q_n *is* $WW(Q_n) = (n+3)n \times 2^{2(n-2)}$.

Proof. Similar to the proof of Theorem 4.4, we put $D(v) = \sum_{x \in V} d(v,x)^2$, hence $WW(Q_n) = \frac{1}{2} W(Q_n) + \frac{1}{4} |V| D(v)$. Now it suffices to calculate $D(v)$. To this end, we may take $v = (0, 0, \dots, 0)$ and calculate $d(v,x)$ for various x. By Lemma 3 in [1], we have $d(v,x) = 1$ if and only if v and x differ in exactly j places. Hence

$$D(v) = \sum_{x \in V} d(v,x)^2 = \sum_{j=1}^{n} j^2 \binom{n}{j} = (n+1)n \times 2^{n-2}$$

by Lemma 5.2. Therefore

$$WW(Q_n) = \frac{1}{2} \times 2^{2(n-1)} n + \frac{1}{4} \times 2^n \times (n+1)n \times 2^{n-2} = (n+3)n \times 2^{2(n-2)}.$$ ■

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REFERENCES

1. M. R. Darafsheh, Computation of topological indices of some graphs, *Acta Appl. Math.* **110** (3) (2010) 1225–1235.
2. M. R. Darafsheh, M. H. Khalifeh and H. Jolany, The hyper-Wiener index of one pentagonal carbon nanocone, *Current Nanoscience* **9** (4) (2013) 557–560.
3. C. Godsil and G. Royle, *Algebraic Graph Theory*, Vol. 207 of Graduate Texts in Mathematics. Springer Verlag, New York – Heidelberg – Berlin, 2001.
4. G. A. Jones, Paley and the Paley graphs, Isomorphisms, symmetry and computations in algebraic graph theory, Springer Proc. Math. Stat., 305, Springer, Cham, (2020) 155–183.

5. M. H. Khalifeh, H. Yousefi-Azari and A. R. Ashrafi, The hyper-Wiener index of graph operations, *Comput. Math. Appl.* **56** (5) (2008) 1402–1407.
6. D. J. Klein, I. Lukovits and I. Gutman, On the definition of the hyper-Wiener index for cycle-containing structures, *J. Chem. Inf. Comput. Sci.* **35** (1995) 50–52.
7. S. M. Mirafzal and M. Ziaee, A note on the automorphism group of the Hamming graph, *Trans. Combin.* **10** (2) (2021) 129–136.
8. R. Modabernia, Some topological indices related to Paley graphs, *Iranian J. Math. Chem.* **11** (2) (2020) 107–112.
9. G. Sabidussi, On a class of fixed-point-free graphs, *Proc. Amer. Math. Soc*. **9** (1958) 800–804.
10. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.