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p-WIENER INTERVALS AND p-WIENER FREE INTERVALS

Kumarappan Kathiresan

Center for Research and Post Graduate Studies in Mathematics
Ayya Nadar Janaki Ammal College
Sivakasi - 626 124, Tamil Nadu, INDIA

e-mail: kathir2esan@yahoo.com

and

S. Arockiaraj

Department of Mathematics
Dr. Sivanthi Aditanar College of Engineering
Tiruchendur-628 215, Tamil Nadu, INDIA

e-mail: sarockiaraj_77@yahoo.com

Abstract

A positive integer n is said to be Wiener graphical, if there exists a graph G with Wiener index n. In this paper, we prove that any positive integer $n(\neq 2,5)$ is Wiener graphical. For any positive integer p, an interval $[a,b]$ is said to be a p-Wiener interval if for each positive integer $n \in [a,b]$ there exists a graph G on p vertices such that $W(G)=n$. For any positive integer p, an interval $[a,b]$ is said to be p-Wiener free interval (p-hyper-Wiener free interval) if there exist no graph G on p vertices with $a \leq W(G) \leq b$ ($a \leq WW(G) \leq b$). In this paper, we determine some p-Wiener intervals and p-Wiener free intervals for some fixed positive integer p.

Keywords: Wiener index of a graph, Wiener graphical, p-Wiener interval, p-Wiener free interval, hyper-Wiener index of a graph, radius, diameter.

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1. Introduction

Throughout this paper, we only concern with connected, undirected simple graphs of order p and size q. Let Γ denote the set of all connected graphs of order p. The distance $d_G(u,v)$ or $d(u,v)$ between the vertices u and v of a graph G is the length of a shortest path that connects u and v. The eccentricity $e(u)$ of a vertex u is the distance to a vertex farthest from u. The radius $r(G)$ of G is the minimum eccentricity among the vertices of G, while the diameter $d(G)$ of G is the maximum eccentricity among the vertices of G. The distance $dist_G(u)$ of a vertex u is $\sum\limits_{v \in V(G)} d_G(u,v)$. The total distance (or just distance) $dist(G)$ of G or the Wiener index $W(G)$ of G is defined as $dist(G) = W(G) = \frac{1}{2} \sum\limits_{u \in V(G)} dist_G(u)$. In other words, $W(G) = \sum\limits_{\{u,v\}} d_G(u,v)$ where the summation is over all unordered pairs $\{u,v\}$ of distinct vertices in G. The hyper-Wiener index $WW(G)$ of G is defined as $WW(G) = \frac{1}{2}(W(G) + \sum\limits_{\{u,v\}} (d_G(u,v))^2)$ where the summation is over all unordered pairs $\{u,v\}$ of distinct vertices in G. The Wiener index $W(G)$ is one of the most frequently applied graph theoretical invariants. It has been used to explain the variation in boiling points, molar volumes, refractive indices, heats of isomerization and heats of vaporization of alkanes [11]. Later heats of formation, atomization, isomerization and vaporization as well as density, critical pressure, surface tension, viscosity, melting points, partition coefficients, chromotographic retention indices and stability of crystal lattices of various kinds of molecules were related to $W(G)$ [6, 10]. Besides chemistry, the concept of Wiener index has been used in electrical engineering [2]. The Wiener index was first proposed by Harold Wiener [11] as an aid to determining the boiling point of paraffin. Since then, the index has been shown to correlate with a host of other properties of molecules (viewed as graphs). It is now recognised that there are good correlations between Wiener index (of molecular graphs) and the physico-chemical properties of the underlying organic compounds. In [7], it was proved that $\frac{p(p-1)}{2} \leq W(G) \leq \frac{p(p^2-1)}{6}$, for any graph G on p vertices and $W(G)$ attains its least and upper bound for $G = K_p$ and $G = P_p$, path on p vertices, respectively. In [9], the first to $(k+1)^{th}$ smallest Wiener indices and the first to $(k+1)^{th}$ smallest hyper-Wiener indices have been found for any two non-negative integers p and k such that $p > 2k$. Motivated by these results, we are very much interested to extend the length of the first to $(k+1)^{th}$ smallest Wiener indices (hyper-Wiener indices) into some extreme. A positive integer n is said to be Wiener graphical, if there exists a graph G with Wiener index n. In this paper, we prove that any positive integer $n (\neq 2, 5)$ is Wiener graphical. For any positive integer p, an interval $[a,b]$ is said to be a p-Wiener interval if for each positive integer $n \in [a,b]$ there exists a graph G on p vertices such that $W(G) = n$. For any positive integer p, an interval $[a,b]$ is said to be p-Wiener free interval (p-hyper-Wiener free interval) if there exist no graph G on p vertices with $a \leq W(G) \leq b$ ($a \leq WW(G) \leq b$). Let F_{11}, F_{12} and F_{22} denote the set of all connected graphs G for which $r(G) = d(G) = 1$; $r(G) = 1$ and $d(G) = 2$ and $r(G) = d(G) = 2$, respectively.

For graph theoretic terminology, we follow [1].

2. Main Results

Lemma 1. *If $G \in F_{11} \cup F_{12}$ and if e is an edge of G such that $G - e \in F_{12}$, then $W(G-e) = W(G) + 1$.*

Proof. For any graph $H \in F_{12}$, $d_H(u,v) = 1$ if and only if $uv \in E(H)$ and $d_H(u,v) = 2$ if and only if $uv \notin E(H)$. Choose an edge $e = xy$ in G so that $G - e \in F_{12}$. For any vertex u other than x and y, we have

$$dist_G(u) = \sum_{v \in V(G)} d_G(u,v) = \sum_{v \in V(G-e)} d_{G-e}(u,v) = dist_{G-e}(u) \text{ and}$$

$$\begin{aligned} dist_G(x) &= \sum_{v \in V(G)} d_G(x,v) = \sum_{v \neq y \in V(G)} d_G(x,v) + d_G(x,y) \\ &= \sum_{v \neq y \in V(G-e)} d_{G-e}(x,v) + d_{G-e}(x,y) - 1 \\ &= \sum_{v \in V(G-e)} d_{G-e}(x,v) - 1 = dist_{G-e}(x) - 1. \end{aligned}$$

Also, $dist_G(y) = dist_{G-e}(y) - 1$. Since $W(G) = \frac{1}{2} \sum\limits_{u \in V(G)} dist_G(u)$, then

$$\begin{aligned} W(G) &= \frac{1}{2}\left(\sum_{u \neq x, u \neq y \in V(G)} dist_G(u) + dist_G(x) + dist_G(y) \right) \\ &= \frac{1}{2}\left(\sum_{u \neq x, u \neq y \in V(G-e)} dist_{G-e}(u) + dist_{G-e}(x) + dist_{G-e}(y) - 2 \right) \\ &= \frac{1}{2}\left(\sum_{u \in V(G-e)} dist_{G-e}(u) - 2 \right) = W(G-e) - 1. \end{aligned}$$ ■

Proposition 2. *For any fixed positive integer $p \geq 2$, $\left[\binom{p}{2}, (p-1)^2 \right]$ is a p-Wiener interval.*

Proof. Clearly, $W(K_p) = \binom{p}{2}$. When $p = 2$, the only connected graph on p vertices is K_2.

For any non-negative integer i, let G_i be a graph obtained from K_p by deleting any i edges other than the $p-1$ edges incident with a particular vertex of K_p. Then $G_i \in F_{12}$ and the maximum possible value of i is $\binom{p-1}{2}$.

By Lemma 1, $W(G_1) = W(K_p) + 1 = \binom{p}{2} + 1$, $W(G_2) = W(G_1) + 1 = \binom{p}{2} + 2$ and so on. The star graph $S_{1,p-1}$ is a member of F_{12} with minimum number of edges which is obtained from K_p by deleting $\begin{pmatrix} p-1 \\ 2 \end{pmatrix}$ edges whose Wiener index is $(p-1)^2$. ■

Proposition 3. *For any positive integer $p \geq 5$, $\left[\frac{p^3-7p+24}{6}, \frac{p^3-p-6}{6}\right]$ is a p-Wiener free interval.*

Proof. The Wiener index $W(G)$ of G attains its maximum when G is a path on p vertices and the next largest value of $W(G)$ is attained when G is a tree obtained from a path $v_1v_2\dots v_{p-1}$ on $p-1$ vertices by attaching a vertex v_p either with the vertex v_2 or with the vertex v_{p-2}. Assume that v_p is attached with v_2. Since the Wiener index of a path on p vertices is $\frac{p(p^2-1)}{6}$,

$$\begin{aligned} W(G) &= W(P_{p-1}) + \sum_{i=1}^{p-1} d_G(v_p, v_i) = W(P_{p-1}) + 2 + 1 + 2 + 3 + \cdots + (p-2) \\ &= \tfrac{(p-1)[(p-1)^2-1]}{6} + 2 + \tfrac{(p-2)(p-1)}{2} = \tfrac{p(p^2-1)}{6} - (p-3) = \tfrac{p^3-7p+18}{6}. \end{aligned}$$ ■

We prove the following proposition using a new construction whose generalisation is used in later discussions.

Proposition 4 [4]**.** *For every positive integer $n (\neq 2, 5)$ in $[(m-1)^2+1, m^2]$, there exists a graph G on $m+1$ vertices with $W(G) = n$.*

Proof. If n is a perfect square, say m^2, then the star graph $S_{1,m}$ is the graph in which $W(S_{1,m}) = m^2$. If n is not a perfect square, then $(m-1)^2 < n < m^2$ for some positive integer $m > 1$. Construct the graph G by adding any (m^2-n) edges in $S_{1,m}$. By applying Lemma 1 successively, we have $W(G) = W(S_{1,m}) - (m^2 - n) = n$. By adding at most $\begin{pmatrix} m \\ 2 \end{pmatrix}$ edges in $S_{1,m}$, we can find a graph to each number n as Wiener index between $(m-1)^2$ and m^2 when $m^2 - [(m-1)^2+1] \leq \begin{pmatrix} m \\ 2 \end{pmatrix}$, that is, when $m^2 - 5m + 4 \geq 0$. $m \geq 4$ is obtained from the fact that $(m-1)(m-4) \geq 0$. When $m = 3, W(S_{1,3}) = 3^2 = 9, W(S_{1,3}+e) = 8$, $W(S_{1,3}+2e) = 7$, $W(S_{1,3}+3e) = W(K_4) = 6$. When G has three vertices, the only connected graphs are K_3 and P_3 whose Wiener indices are 3 and 4 respectively. The Wiener indices fall on $[1,1]$, $[3,4]$, $[6,10]$, $[10,20]$ etc., when the number of vertices are 2, 3, 4, 5 etc., respectively. So we cannot find a graph G with Wiener index either 2 or 5. ■

Theorem 5. *For any fixed positive integer $p \geq 4$, $\left[\binom{p}{2}, (p-1)^2 + k(p-3)\right]$ is a p-Wiener interval, where $k = \left\lfloor \frac{2p-3-\sqrt{8p-31}}{4} \right\rfloor$.*

Proof. When $p \geq 4$, we may obtain that $\left[\binom{p}{2}, (p-1)^2\right]$ is a p-Wiener interval as in Proposition 2 and the upper bound is obtained when $G = S_{1,p-1}$, the star graph on p vertices.

Let $v_1, v_2, \ldots, v_{p-1}$ be the pendent vertices and v_p be the vertex of degree $p-1$ of the star graph $S_{1,p-1}$. Let G_k be the graph obtained from $S_{1,p-1}$ by deleting the edges $v_2v_p, v_4v_p, \ldots, v_{2k}v_p$ and adding the new edges $v_1v_2, v_3v_4, \ldots, v_{2k-1}v_{2k}$.

In G_k, $dist_{G_k}(v_{2i-1}) = 2 + 5(k-1) + 2(p-2k-1) = 2p + k - 5$ and $dist_{G_k}(v_{2i}) = 1 + 2 + 7(k-1) + 3(p-2k-1) = 3p + k - 7$, for $1 \leq i \leq k$. For $2k+1 \leq i \leq p-1$, $dist_{G_k}(v_i) = 1 + 2(p-2k-2) + 5k = 2p + k - 3$ and $dist_{G_k}(v_p) = p - 2k - 1 + 3k = p + k - 1$. Hence $W(G_k) = \frac{1}{2}\sum\limits_{i=1}^{p} dist_{G_k}(v_i)$

$$= \frac{1}{2}\left(\sum_{i=1}^{k}(dist_{G_k}(v_{2i-1}) + dist_{G_k}(v_{2i})) + \sum_{i=2k+1}^{p-1} dist_{G_k}(v_i) + dist_{G_k}(v_p)\right)$$

$$= \frac{1}{2}\left(\sum_{i=1}^{k}(5p + 2k - 12) + \sum_{i=2k+1}^{p-1}(2p + k - 3) + p + k - 1\right) = (p-1)^2 + k(p-3).$$

Also $[W(G_{k-1}), W(G_k)]$ is a closed interval of length $p-3$, where $G_0 = S_{1,p-1}$. By adding $p-4$ edges one by one in G_k like $v_{2k+1}v_{2k+2}, v_{2k+1}v_{2k+3}, \ldots, v_{2k+1}v_{p-1}$, $v_{2k+2}v_{2k+3}, v_{2k+2}v_{2k+4}, \ldots, v_{2k+2}v_{p-1}$ and so on, corresponding $p-4$ new graphs $G_k^1, G_k^2, \ldots, G_k^{p-4}$ are obtained in which $W(G_k^1) = W(G_k) - 1$, $W(G_k^{i+1}) = W(G_k^i) - 1$, for $1 \leq i \leq p-5$ and $W(G_{k-1}) = W(G_k^{p-4}) - 1$. Similarly, for any $1 \leq j \leq k-1$, $W(G_{k-j}^1) = W(G_{k-j}) - 1$, $W(G_{k-j}^{i+1}) = W(G_{k-j}^i) - 1$, for $1 \leq i \leq p-5$ and $W(G_{k-j-1}) = W(G_{k-j}^{p-4}) - 1$. The above is possible when $\binom{p-2k-1}{2} \geq p-4$. From this, the suitable and largest value of k is $\left\lfloor \frac{2p-3-\sqrt{8p-31}}{4} \right\rfloor$. ■

Now our attention is on the hyper-Wiener index of graphs.

Proposition 6. *If $G \in F_{11} \cup F_{12} \cup F_{22}$, then $WW(G) = 3\binom{p}{2} - 2q$.*

Proof. Since $G \in F_{11} \cup F_{12} \cup F_{22}, d_G(u,v) = 1$ if and only if $uv \in E(G)$ and $d_G(u,v) = 2$ if and only if $uv \notin E(G)$. Hence

$$\begin{aligned} WW(G) &= \frac{1}{2}\left(\sum_{\{u,v\}\subseteq V(G)} d_G(u,v) + \sum_{\{u,v\}\subseteq V(G)} (d_G(u,v))^2\right) \\ &= \frac{1}{2}\left(\left(q + 2\left(\binom{p}{2} - q\right)\right) + \left(q + 4\left(\binom{p}{2} - q\right)\right)\right) \\ &= \frac{1}{2}\left(6\binom{p}{2} - 4q\right) = 3\binom{p}{2} - 2q. \end{aligned}$$

■

Note that for $G = K_p$, by Proposition 6, $WW(G) = \binom{p}{2} = W(G)$.

Theorem 7. *For any fixed positive integer $p \geq 2$, there exists a graph G_i in Γ such that $WW(G_i) = \binom{p}{2} + 2i$, for all $0 \leq i \leq \binom{p-1}{2}$.*

Proof. If e is an edge of G of order p and size q in which $G - e \in F_{12}$, then by Proposition 6, $WW(G - e) = 3\binom{p}{2} - 2(q-1) = WW(G) + 2$.

When $p = 2$, the only connected graph on p vertices is K_2 whose hyper-Wiener index is $\binom{p}{2}$. For any non-negative integer i, let G_i be a graph obtained from K_p by deleting any i edges other than the $p-1$ edges incident with a particular vertex of K_p. Then $WW(G_1) = WW(K_p - e_1) = \binom{p}{2} + 2$, $WW(G_2) = WW(G_1 - e) = WW(G_1) + 2 = \binom{p}{2} + 4$ and so on. In general, $WW(G_i) = \binom{p}{2} + 2i$, for all $0 \leq i \leq \binom{p-1}{2}$. ■

It is easy to verify that the hyper-Wiener index of a tree T attains its minimum value $\frac{3p(p-1)}{2}$ when $T = S_{1,p-1}$, the star graph on p vertices and attains its maximum value $\frac{p(p^2-1)(p+2)}{24}$ when T is a path on p vertices. Using this, we have found a p-hyper-Wiener free interval in the following proposition.

Proposition 8. *For any positive integer $p \geq 5$, $\left[\frac{p^4+2p^3-13p^2+10p+96}{24}, \frac{p^4+2p^3-p^2-2p-24}{24}\right]$ is a p-hyper-Wiener free interval.*

Proof. The hyper-Wiener index $WW(G)$ of G attains its maximum when G is a path on p vertices and the next largest value of $WW(G)$ is attained on G when G is a tree obtained from a path $v_1v_2\ldots v_{p-1}$ on $p-1$ vertices by attaching the vertex v_p either with the vertex v_2 or with vertex v_{p-2}. If v_p is attached with v_2, then it can be shown that $WW(G) = \frac{p^4+2p^3-13p^2+10p+72}{24}$ from the definition of hyper-Wiener index and by the part of the proof in Proposition 3. ■

Problem for Further Study: For any positive integer p, we are able to produce some graphs with p vertices whose Wiener index is in the interval $\left[(p-1)^2 + k(p-3) + 1, \frac{p^3-7p+12}{6}\right]$, where $k = \left\lfloor \frac{2p-3-\sqrt{8p-31}}{4} \right\rfloor$. The problem of deciding which subintervals of the above interval are p-Wiener intervals or not is still open.

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$\left[p^2 - p - 1, \frac{p^3-7p+18}{6}\right]$. By the suggestions given by one of the referees, we reduce this interval into $\left[(p-1)^2 + k(p-3) + 1, \frac{p^3-7p+12}{6}\right]$, where $k = \left\lfloor \frac{2p-3-\sqrt{8p-31}}{4} \right\rfloor$. We thank the referees for their encouraging comments on this paper.

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