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On the extremal hyper-wiener index of graphs

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ABSTRACT

In this paper, we consider the relationship between Hyper-Wiener index and some special parameters of graph, and present the graphs which minimize the Hyper-Wiener index among all graphs with given chromatic number and clique number and the graphs which maximum the Hyper-Wiener index among all graphs with given chromatic number and clique number.

Keywords: Chemical graph theory, organic molecules, Hyper-Wiener index, chromatic number, clique number

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INTRODUCTION

The Hyper-Wiener index, as an extension of Wiener index, is an important topological index in Chemistry. It is used for the structure of molecule. There is a very close relation between the physical, chemical characteristics of many compounds and the topological structure of that. The Hyper-Wiener index is such a topological index and it has been widely used in Chemistry fields. Some conclusion for Hyper-Wiener index can refer to [1].

The graphs considered in this paper are simple and connected. The vertex and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. The Wiener index is defined as the sum of distances between all unordered pair of vertices of a graph G, i.e.,

$$W(G)=\sum_{\{u,v\}\subseteq V(G)} d(u,v),$$

where $d(u,v)$ is the distance between u and v in G.

Several papers contributed to determine the Wiener index of special graphs. Gao and Shi [2] determined the Wiener index of gear fan graph, gear wheel graph and their r-corona graphs. Chen [3]gained the exact expression for general pepoid graph. Xing and Cai [4] characterized the tree with third-minimum wiener index and introduce the method of obtaining the order of the Wiener indices among all the trees with given order and diameter, respectively. A tricyclic graph is a connected graph with n vertices and n+2 edges. Wan and Ren [5] studied the Wiener index of tricyclic graph τ_n^3 which have at most a common vertex between any two circuits, and the smallest, the second-smallest Wiener indices of the tricyclic graphs τ_n^3 are given. The Hyper-Wiener index WW is one of the recently distance-based graph invariants. That WW clearly encodes the compactness of a structure and the WW of G is define as:

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

Pan [6] deduced the formula of Wiener number and Hyper-Wiener number of two types of polyomino systems. More results on Wiener index and Hyper-Wiener index can refer to [7-14].

In this paper, we connect the Hyper-Wiener index with some well-known graph theoretic parameters, such as chromatic number and clique number. It is proved that among all graphs with *n* vertices and chromatic number *k*, the Hyper-Wiener index is minimized by the graph $T_{k,n}$, and among all graphs with *n* vertices and clique number *k*, the Hyper-Wiener index is minimized by the graph $T_{k,n}$ and maximized by the graph $K_k \cdot P_{n-k}$. Note that $T_{k,n}$ is complete *k*-partite graph on *n* vertices in which each part has either $\lfloor n/k \rfloor$ or $\lceil n/k \rceil$ vertices. Let $\chi(G)$ and $c(G)$ be the chromatic number and clique number of graph *G*, respectively.

1. Main results and proof

Theorem 1. Let *G* be a graph on *n* vertices and with $\chi(G)=k$. Let $t=\lfloor n/k \rfloor$. Then

$$WW(G) \ge \frac{3n(n-1)}{2} - 2\binom{n-t}{2} - 2(k-1)\binom{t+1}{2} \tag{1}$$

and the equality holds if and only if $G \cong T_{k,n}$.

Proof. Let G^* be a graph with minimum Hyper-Wiener index in all graphs with *n* vertices and chromatic number *k*. Then the vertex set of G^* can be divided into *k* parts such that no edges joins two vertices from same part. Moreover, G^* includes all edges joining vertices in different parts. Otherwise, there exists two disconnect vertices *v* and *v*' which belong to different parts. Then the graph G^*+vv' has chromatic number *k* and fewer Hyper-Wiener index than G^*, which contradicts to the selection of G^*. Hence, G^* is a complete *k*-partite graph $K_k(r_1, r_2, \cdots, r_k)$ with $r_1+r_2+\cdots+r_k=n$,where r_i is the number of vertex in *i*-th part ($1 \le i \le k$).

We now claim that $G^* \cong T_{k,n}$. Otherwise, the parts are not as equal as possible, suppose there are r_i vertices in the *i*-th part and $r_j \ge r_i + 2$ in the *j*-th part. Then by transferring one vertex from the *j*-th part to the *i*-th part, the Hyper-Wiener index will decrease which contradicts to the selection of G^*.

Since $|E(T_{k,n})| = \binom{n-t}{2} + (k-1)\binom{t+1}{2}$. We have

$$WW(T_{k,n}) = \frac{1}{2}\Big(\sum_{\{u,v\}\subseteq V(T_{k,n})} d(u,v)^2 + \sum_{\{u,v\}\subseteq V(T_{k,n})} d(u,v)\Big)$$
$$= \frac{1}{2}\Big\{\Big(4\binom{n}{2} - 3\Big[\binom{n-t}{2} + (k-1)\binom{t+1}{2}\Big]\Big) + \Big(2\binom{n}{2} - \Big[\binom{n-t}{2} + (k-1)\binom{t+1}{2}\Big]\Big)\Big\}$$
$$= \frac{3n(n-1)}{2} - 2\binom{n-t}{2} - 2(k-1)\binom{t+1}{2}.$$

The proof above implies that equality holds in (1) if and only if $G \cong T_{k,n}$. The Theorem thus follows. □

Our second result depends heavily on the following lemma.

Lemma 1. [15] Let *G* be a graph on *n* vertices. If *G* contains on K_{m+1}, then $|E(G)| \le |E(T_{k,n})|$. Moreover, $|E(G)| = |E(T_{k,n})|$ only if $G \cong T_{k,n}$.

Since for $c(G)=n$ or n-1, it is not hard to obtain the lower bound and upper bound on Hyper-Wiener index. In following theorem, we only consider the graph G on n vertices with clique number $c(G)<n-1$. Let $d(G,i)$ be the number of vertex pairs at distance i. Let $K_k \cdot P_{n-k}$ be the graph obtained from K_k and P_{n-k} by joining a vertex of K_k to one end vertex of P_{n-k}.

Theorem 2. Let G be a graph on n vertices with clique number $c(G)=k<n-1$. Then, we have

$$\frac{3n(n-1)}{2} - 2\binom{n-t}{2} - 2(k-1)\binom{t+1}{2} \le WW(G)$$
$$\le \frac{1}{2}((\binom{k}{2} + \sum_{i=1}^{n-k}(n-k-i+1)i^2 + (k-1)\sum_{i=2}^{n-k+1} i^2)$$
$$+(\binom{k}{2} + \binom{n-k+1}{3} + (k-1)[\frac{(n-k+1)(n-k+2)}{2} - 1] + \frac{(n-k)(n-k+1)}{2}))$$

where $t=\lfloor n/k \rfloor$. Moreover, the lower bound is achieved if and only if $G \cong T_{k,n}$ and the upper bound is achieved if and only if $G \cong K_k \cdot P_{n-k}$.

Proof. Let G be a graph on n vertices with clique number $c(G)=k<n-1$ and l be the diameter of G. Then, in terms of Lemma 1, we get

$$WW(G) = \frac{1}{2}(\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2 + \sum_{\{u,v\}\subseteq V(G)} d(u,v))$$
$$= \frac{1}{2}((|E(G)| + \sum_{i=2}^{l} i^2 d(G,i)) + (|E(G)| + \sum_{i=2}^{l} i d(G,i)))$$
$$\ge \frac{1}{2}((|E(G)| + 4\sum_{i=2}^{l} d(G,i)) + (|E(G)| + 2\sum_{i=2}^{l} d(G,i))) \tag{2}$$
$$= \frac{1}{2}((|E(G)| + 4[\binom{n}{2} - |E(G)|]) + (|E(G)| + 2[\binom{n}{2} - |E(G)|]))$$
$$= 3\binom{n}{2} - 2|E(G)|$$
$$\ge \frac{3n(n-1)}{2} - 2|E(T_{k,n})| \tag{3}$$
$$= \frac{3n(n-1)}{2} - 2\binom{n-t}{2} - 2(k-1)\binom{t+1}{2}.$$

It is fact that equality in both (2) and (3) will hold if and only if $G \cong T_{k,n}$. Note that the clique number of graph $T_{k,n}$ is k. Hence, we obtain

$$WW(G) \ge \frac{3n(n-1)}{2} - 2\binom{n-t}{2} - 2(k-1)\binom{t+1}{2},$$

and the equality holds if and only if $G \cong T_{k,n}$.

In the following, we will prove the upper bound on Hyper-Wiener index by induction on vertex number n.

Let G^* be a graph with maximum Hyper-Wiener index in all graphs with n vertices and clique number $k<n-1$.

Clearly, G^* has a pendent vertex, say u. Let v be the pendent vertex of $K_k \cdot P_{n-k}$. Then, we infer

$$WW(G^*) = WW(G^* - u) + d_{G^*}(u),$$
$$WW(K_k \cdot P_{n-k}) = WW(K_k \cdot P_{n-k} - v) + d_{K_k \cdot P_{n-k}}(v).$$

Obviously, G^*-u has n-1 vertices and with clique number k. In view of induction hypothesis, we deduce $WW(G^* - u) \le WW(K_k \cdot P_{n-k} - v)$. Since $d_{G^*}(u) \le d_{K_k \cdot P_{n-k}}(v)$ and the equality holds if and only if $G \cong K_k \cdot P_{n-k}$. We yield $WW(G^*) \le WW(K_k \cdot P_{n-k})$.

By straightforward calculation, we have

$$WW(K_k \cdot P_{n-k}) = \frac{1}{2}\Big(\sum_{\{u,v\} \subseteq V(K_k \cdot P_{n-k})} d(u,v)^2 + \sum_{\{u,v\} \subseteq V(K_k \cdot P_{n-k})} d(u,v)\Big)$$

$$= \frac{1}{2}\Big(\Big(\binom{k}{2} + \sum_{i=1}^{n-k}(n-k-i+1)i^2 + (k-1)\sum_{i=2}^{n-k+1} i^2\Big)$$

$$+\Big(\binom{k}{2} + \binom{n-k+1}{3} + (k-1)\Big[\frac{(n-k+1)(n-k+2)}{2} - 1\Big] + \frac{(n-k)(n-k+1)}{2}\Big)\Big).$$

Thus,

$$WW(G) \le \frac{1}{2}\Big(\Big(\binom{k}{2} + \sum_{i=1}^{n-k}(n-k-i+1)i^2 + (k-1)\sum_{i=2}^{n-k+1} i^2\Big)$$

$$+\Big(\binom{k}{2} + \binom{n-k+1}{3} + (k-1)\Big[\frac{(n-k+1)(n-k+2)}{2} - 1\Big] + \frac{(n-k)(n-k+1)}{2}\Big)\Big).$$

and the proof above reveals that the equality holds if and only if $G \cong K_k \cdot P_{n-k}$. □

CONCLUSION

The contributions of our paper are determining the upper bound and lower bound of Hyper-Wiener index under fixed chromatic number and clique number. Our results also present the sufficient and necessary condition for reaching the upper and lower bound.

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