A theorem on Wiener-type invariants for isometric subgraphs of hypercubes

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Abstract
Let \( d(G, k) \) be the number of pairs of vertices of a graph \( G \) that are at distance \( k \), \( \lambda \) a real (or complex) number, and \( W_\lambda(G) = \sum_{k \geq 1} d(G, k) k^\lambda \). It is proved that for a partial cube \( G \), \( W_{\lambda+1}(G) = |F| W_\lambda(G) - \sum_{F \subseteq \mathcal{F}} W_\lambda(G \setminus F) \), where \( \mathcal{F} \) is the partition of \( E(G) \) induced by the Džoković-Winkler relation \( \Theta \). This result extends previously known result for trees and implies several relations for distance-based topological indices.

Key words: graph distance, hypercube, partial cube, Wiener number, hyper-Wiener index.

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1 Introduction

The **Wiener number** (or **Wiener index**) \( W(G) \) of a connected graph \( G \) is the sum of distances between all pairs of vertices of \( G \), that is,

\[
W(G) = \sum_{\{u,v\} \subseteq V(G) \times V(G)} d(u, v).
\]
In the case of trees the Wiener number was introduced back in 1947 by Wiener in [25], hence the name of this graph invariant. Until today, it has been extensively investigated, above all in mathematical chemistry, see special issues of journal devoted to the topic [13, 14], recent surveys [5, 6], and recent papers [7, 8, 9].

The Wiener number can be extended to disconnected graphs as follows [12]. Denote by \( d(G, k) \) the number of pairs of vertices of \( G \) that are at distance \( k \). Note that \( d(G, 0) \) and \( d(G, 1) \) represent the number of vertices and edges, respectively. Then \( W \) can be extended to disconnected graphs as

\[
W(G) = \sum_{k \geq 1} d(G, k) k^\lambda,
\]

where \( \lambda \) is some real (or complex) number. Several particular instances of the invariant \( W_\lambda \) have been previously studied. For instance, \( W_{-2} \), \( W_{-1} \), \( \frac{1}{2} W_1 \), and \( \frac{1}{2} W_3 + \frac{1}{2} W_2 + \frac{1}{3} W_1 \) are the so-called Harary index, reciprocal Wiener index, hyper–Wiener index, and Tratch-Stankevich-Zefirov index, cf. [12] and references therein. In the chemical literature also \( W_{1/2} \) [27] as well as the general case \( W_\lambda \) were examined [10, 11, 15].

Let \( T \) be a tree, then in [12] the following recursive formula for \( W_\lambda \) has been obtained:

\[
W_{\lambda+1}(T) = (n - 1) W_\lambda(T) - \sum_{e \in E(T)} W_\lambda(T - e). \tag{1}
\]

In this note we prove that if \( G \) is a partial cube and \( \mathcal{F} \) the partition of \( E(G) \) induced by the Djoković-Winkler relation \( \Theta \), then

\[
W_{\lambda+1}(G) = |\mathcal{F}| W_\lambda(G) - \sum_{F \in \mathcal{F}} W_\lambda(G \setminus F). \tag{2}
\]

Since trees are partial cubes in which the partition \( \mathcal{F} \) is trivial, that is, every edge of a tree forms a class of the partition, (1) immediately follows from (2). In addition we will demonstrate that some known relations between distance-based topological indices follow from formula (2).

2 The main result

For \( u, v \in V(G) \), let \( d_G(u, v) \) denote the length of a shortest path (also called geodesic) in \( G \) from \( u \) to \( v \). A subgraph \( H \) of a graph \( G \) is called isometric if \( d_H(u, v) = d_G(u, v) \) for all \( u, v \in V(H) \). Isometric subgraphs of hypercubes are called partial cubes. Clearly, hypercubes are partial cubes, as well as are trees and median graphs. Partial cubes form a well studied class of graphs, we refer to classical references [1, 4, 26], book [16], recent paper [20] and references therein. For applications of partial cubes to mathematical chemistry see [3, 17, 18, 19, 21].
The Djoković-Winkler relation Θ is defined on the edge set of a graph in the following way [4, 26]. Edges \( e = xy \) and \( f = uv \) of a graph \( G \) are in relation Θ if

\[
d_G(x, u) + d_G(y, v) \neq d_G(x, v) + d_G(y, u).
\]

Winkler [26] proved that among bipartite graphs, Θ is transitive precisely for partial cubes, hence Θ partitions the edge set of a partial cube. Let \( G \) be a partial cube and \( \mathcal{F} = \{F_1, F_2, \ldots, F_r\} \) the partition of its edge set induced by the relation Θ. Then we say that \( \mathcal{F} \) is the Θ-partition of \( G \).

For the proof of our main theorem we need the following facts about Θ, cf. [16, 20].

**Lemma 1** Let \( G \) be a partial cube.

(i) A path \( P \) in \( G \) is a geodesic if and only if no two different edges of \( P \) are in relation Θ.

(ii) Let \( F \) be a class of the Θ-partition of \( G \). Then \( G \setminus F \) consists of two connected components.

We are now ready for our main result.

**Theorem 2** Let \( G \) be a partial cube and \( \mathcal{F} \) its Θ-partition. Then for any real (or complex) number \( \lambda \),

\[
W_{\lambda+1}(G) = |\mathcal{F}| W_\lambda(G) - \sum_{F \in \mathcal{F}} W_\lambda(G \setminus F).
\]

**Proof.** Let \( s \) be the diameter of \( G \), then

\[
W_\lambda(G) = \sum_{k=1}^{s} d(G, k) k^\lambda.
\]

Let \( \mathcal{F} = \{F_1, F_2, \ldots, F_r\} \) and set

\[
X = \sum_{i=1}^{r} W_\lambda(G \setminus F_i).
\]

Let \( u \) and \( v \) be arbitrary vertices of \( G \), where \( d(u, v) = k, 1 \leq k \leq s \). Let \( P \) be a \( u, v \)-geodesic. By Lemma 1 (i), the edges of \( P \) belong to pairwise different classes of \( \mathcal{F} \). We may assume without loss of generality that they belong to \( F_1, F_2, \ldots, F_k \). By Lemma 1 (ii), \( u \) and \( v \) belong to different connected components of \( G \setminus F_i \) for \( i = 1, \ldots, k \). On the other hand, \( u \) and \( v \) are in the same connected component of \( G \setminus F_i \) for \( i = k + 1, \ldots, r \). Clearly, in the latter case, \( d_{G \setminus F_i}(u, v) = k \). It follows that the pair \( \{u, v\} \) contributes \( (r - k) \)-times to \( X \). Thus,

\[
X = \sum_{k=1}^{s} (r - k) d(G, k) k^\lambda
\]

\[
= r \sum_{k=1}^{s} d(G, k) k^\lambda - \sum_{k=1}^{s} d(G, k) k^{\lambda+1}
\]

\[
= r W_\lambda(G) - W_{\lambda+1}(G).
\]
If $F$ is a $\Theta$-class of the hypercube $Q_n$, then $Q_n \setminus F$ consists of two disjoint copies of $Q_{n-1}$. Thus, by Theorem 2, $W_{\lambda+1}(Q_n) = nW_\lambda(Q_n) - 2nW_\lambda(Q_{n-1})$. By this recurrence relation it follows that $W_\lambda(Q_n) = p_\lambda(n)4^n$, where $p_\lambda(n)$ is a polynomial. This can also be seen from the formula $W_\lambda(Q_n) = 2^{n-1} \sum_{k=1}^{n} \binom{n}{k} k^\lambda$.

3 Applications

In this section we give two applications of Theorem 2. The first one is the following result for the Wiener number, first given in [19], and extended to the so-called $L_1$-graphs in [2].

Let $G$ be a partial cube, $\mathcal{F}$ its $\Theta$-partition, and $F \in \mathcal{F}$. Then we will denote the connected components of $G \setminus F$ by $G_1(F)$ and $G_2(F)$. Set $n_1(F) = |G_1(F)|$ and $n_2(F) = |G_2(F)|$.

**Corollary 3** Let $G$ be a partial cube and $\mathcal{F}$ its $\Theta$-partition. Then

$$W_1(G) = W(G) = \sum_{F \in \mathcal{F}} n_1(F) n_2(F).$$

**Proof.** Let $n = |V(G)|$, then for any $F \in \mathcal{F}$, $n_1(F) + n_2(F) = n$. Using Theorem 2 we can compute as follows.

$$W_1(G) = |\mathcal{F}|W_0(G) - \sum_{F \in \mathcal{F}} W_0(G \setminus F)$$

$$= |\mathcal{F}| \binom{n}{2} - \sum_{F \in \mathcal{F}} \left[ \binom{n_1(F)}{2} + \binom{n_2(F)}{2} \right]$$

$$= |\mathcal{F}| \binom{n}{2} - \frac{1}{2} \sum_{F \in \mathcal{F}} \left[ n^2 - n - 2n_1(F)n_2(F) \right]$$

$$= |\mathcal{F}| \binom{n}{2} - \frac{1}{2} \sum_{F \in \mathcal{F}} (n^2 - n) + \sum_{F \in \mathcal{F}} n_1(F)n_2(F)$$

$$= \sum_{F \in \mathcal{F}} n_1(F)n_2(F).$$

For the second application some more concepts are needed. The hyper-Wiener index $WW$ is a topological index proposed by Randić [24] for trees and extended to all graphs by Klein, Lukovits, and Gutman [22] as

$$WW(G) = \frac{1}{2}W_1(G) + \frac{1}{2}W_2(G).$$
Let $G$ be a partial cube, $\mathcal{F}$ its $\Theta$-partition, and $F,F' \in \mathcal{F}, F \neq F'$. Then we will denote $n_{11}(F,F') = |G_1(F) \cap G_1(F')|$, $n_{12}(F,F') = |G_1(F) \cap G_2(F')|$, $n_{21}(F,F') = |G_2(F) \cap G_1(F')|$, and $n_{22}(F,F') = |G_2(F) \cap G_2(F')|$. We say that the classes $F$ and $F'$ cross if $n_{k\ell}(F,F') \neq 0$ for $1 \leq k, \ell \leq 2$, and write $F \neq F'$ to denote the fact that $F$ and $F'$ cross, see [20, 23]. Now we can deduce from Theorem 2 the following result given in [17].

**Corollary 4** Let $G$ be a partial cube and $\mathcal{F} = \{F_1, F_2, \ldots, F_r\}$ its $\Theta$-partition. Then

$$WW(G) = W(G) + \sum_{i<j} [n_{11}(F_i, F_j) n_{22}(F_i, F_j) + n_{12}(F_i, F_j) n_{21}(F_i, F_j)].$$

**Proof.** By Theorem 2, $W_2(G) = rW(G) - \sum_{i=1}^r W(G \setminus F_i)$. On the other hand, $WW(G) = W(G)/2 + W_2(G)/2$. Combining these two equalities we get

$$WW(G) = W(G) + \frac{1}{2} \left[ (r-1)W(G) - \sum_{i=1}^r W(G \setminus F_i) \right].$$

By Corollary 3 we have

$$(r-1)W(G) = \sum_{j=1}^{r-1} \sum_{i=1}^r n_1(F_i) n_2(F_i) = \sum_{i=1}^r \sum_{j=1}^{r-1} n_1(F_i) n_2(F_i),$$

while on the other hand

$$\sum_{i=1}^r W(G \setminus F_i) = \sum_{i=1}^r [W(G_1(F_i)) + W(G_2(F_i))].$$

Combining (4) and (5) with (3) we obtain:

$$WW(G) = W(G) + \frac{1}{2} \sum_{i=1}^r \left[ \sum_{j=1}^{r-1} n_1(F_i) n_2(F_i) - W(G_1(F_i)) - W(G_2(F_i)) \right].$$

Having in mind Corollary 3 we now consider the contribution of a fixed pair of classes $F_i$ and $F_j$ to the right-hand side sum in (6). For the rest of the proof let $n_{11}, n_{12}, n_{21},$ and $n_{22}$ denote $n_{11}(F_i, F_j)$, $n_{12}(F_i, F_j)$, $n_{21}(F_i, F_j)$, and $n_{22}(F_i, F_j)$, respectively.

Suppose first that $F_i$ and $F_j$ cross. Then the contribution of the pair $F_i, F_j$ is

$$\left[(n_{11} + n_{12})(n_{21} + n_{22}) + (n_{11} + n_{21})(n_{12} + n_{22})\right] - \left[(n_{11}n_{12} + n_{21}n_{22})

+(n_{11}n_{21} + n_{12}n_{22})\right] = 2n_{11}n_{22} + 2n_{12}n_{21}.$$
(i) \((n_{11} + n_{12})n_{22} + n_{11}(n_{12} + n_{22}) - (n_{11}n_{12} + n_{12}n_{22}) = 2n_{11}n_{22},\)

(ii) \((n_{11} + n_{12})n_{21} + n_{12}(n_{11} + n_{21}) - (n_{12}n_{11} + n_{11}n_{21}) = 2n_{12}n_{21},\)

(iii) \((n_{21} + n_{22})n_{11} + n_{22}(n_{11} + n_{21}) - (n_{21}n_{22} + n_{21}n_{11}) = 2n_{11}n_{22},\)

(iv) \((n_{21} + n_{22})n_{12} + n_{21}(n_{12} + n_{22}) - (n_{21}n_{22} + n_{22}n_{21}) = 2n_{12}n_{21}.\)

Since in cases (i), (ii), (iii), and (iv) we have \(n_{21} = 0, n_{22} = 0, n_{12} = 0,\) and \(n_{11} = 0,\) respectively, in all cases the contribution of \(F_i\) and \(F_j\) to the right-hand side sum in (6) can be written as

\[2n_{11}n_{22} + 2n_{12}n_{21}\]

which completes the argument. \(\square\)

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References


