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WIENER INVARIANTS OF PRODUCT OF GRAPHS

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ABSTRACT. The Wiener index of a connected graph Λ, denoted by $W(\Lambda)$, is defined as $\frac{1}{2}\sum\limits_{u,\,v\,\in\,V(\Lambda)} dist_\Lambda(u,v)$. In this paper, we present the explicit formulae for the Wiener invariant of tensor product of a given graph and a complete bipartite graph.

1. INTRODUCTION

A topological invariant is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph. A representation of an object giving information only about the number of elements composing it and their connectivity is named as topological representation of an object. One of the most widely known topological descriptor is the Wiener invariant named after chemist Harold Wiener. The Wiener invariant [2] of a graph is defined as $W(\Lambda) = \frac{1}{2}\sum\limits_{u,\,v\,\in\,V(\Lambda)} dist_\Lambda(u,v)$.

The reverse Wiener invariant was proposed by Balaban et al. in 2000 [3], it turns out that this invariant is important for a reverse problem and also found applications in modeling of structure-property relations [3, 4]. The reverse-Wiener invariant is defined as follows $\Lambda(\Lambda) = \frac{1}{2}n(n-1)D(\Lambda) - W(\Lambda)$, where n is the number of vertices and $D(\Lambda)$ is the diameter of Λ. Some mathematical properties of the reverse Wiener invariant may be found in [5–7].

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The chemical applications and mathematical properties of the Wiener invariant are well studied in [1]. Pattabiraman and Paulraja [8] have obtained the Wiener type invariants of tensor product of a connected graph and complete $r-$ partite graph with $r \geq 3$. In this paper, the formulae for Wiener and reverse Wiener invariants of tensor product of a connected graph and complete bipartite graphs are obtained.

2. WIENER INVARIANT

Let Λ be a connected graph with $V(\Lambda) = \{v_0, v_1, \ldots, v_{n-1}\}$ and let $K_{a,b}$ be the complete bipartite graph with partite sets V_0, V_1 and let $|V_0| = a$, $|V_1| = b$. In the graph $\Lambda \times K_{a,b}$, let $B_{ij} = v_i \times V_j, v_i \in V(\Lambda)$ and $j = 0, 1$. The proof of the following lemma is follows from the structure of the graph $\Lambda \times K_{a,b}$.

Lemma 2.1. *Let Λ be a graph on n vertices with each edge of Λ is on a triangle. The distances between B_{ij} to B_{kp} in $\mathscr{B}$ of the graph $H = \Lambda \times K_{a,b}$ as follows:*

(i) $dist_H(B_{i0}, B_{i1}) = dist_H(B_{i1}, B_{i0}) = 3ab.$

(ii) *If* $v_iv_k \in E(\Lambda)$, *then* $dist_H(B_{i0}, B_{k0}) = 2a^2$ *and* $dist_H(B_{i1}, B_{k1}) = 2b^2.$

(iii) *If* $v_iv_k \notin E(\Lambda)$, *then*

$$dist_H(B_{i0}, B_{k0}) = \begin{cases} a^2\, dist_\Lambda(v_i, v_k), & \text{if } dist_\Lambda(v_i, v_k) \text{ is even} \\ a^2\left(dist_\Lambda(v_i, v_k) + 1\right), & \text{if } dist_\Lambda(v_i, v_k) \text{ is odd} \end{cases}$$

$$dist_H(B_{i1}, B_{k1}) = \begin{cases} b^2\, dist_\Lambda(v_i, v_k), & \text{if } dist_\Lambda(v_i, v_k) \text{ is even} \\ b^2\left(dist_\Lambda(v_i, v_k) + 1\right), & \text{if } dist_\Lambda(v_i, v_k) \text{ is odd} \end{cases}$$

and

$$dist_H(B_{i0}, B_{k1}) = dist_H(B_{i1}, B_{k0})$$
$$= \begin{cases} ab\, dist_\Lambda(v_i, v_k), & \text{if } dist_\Lambda(v_i, v_k) \text{ is odd} \\ ab\left(dist_\Lambda(v_i, v_k) + 1\right), & \text{if } dist_\Lambda(v_i, v_k) \text{ is even.} \end{cases}$$

(iv) $dist_H(B_{i0}, B_{i0}) = 2a(a-1)$ *and* $dist_H(B_{i1}, B_{i1}) = 2b(b-1).$

Let ℓ_1(resp. ℓ_2) denote the number of (unordered) pairs of vertices which are at an odd(resp. even) distances in Λ. Now we obtain the Wiener invariant of $\Lambda \times K_{a,b}$.

Theorem 2.1. *If Λ is a graph on n vertices with each edge of Λ is on a triangle, then $W(\Lambda \times K_{a,b}) = (a+b)^2 W(\Lambda) + (a^2+b^2)\ell_1 + ab(3n+2\ell_2) + n(a^2+b^2-a-b)$, where ℓ_1 and ℓ_2 are as defined above.*

Proof. Let $H = \Lambda \times K_{a,b}$. By the definition of Wiener index

$$\begin{aligned}
W(H) &= \frac{1}{2} \sum_{B_{ij}, B_{kp} \in \mathscr{B}} dist_H(B_{ij}, B_{kp}) \\
&= \frac{1}{2}\Big(\sum_{i=0}^{n-1} \sum_{\substack{j,p=0 \\ j \neq p}}^{1} dist_H(B_{ij}, B_{ip}) + \sum_{\substack{i,k=0 \\ i \neq k}}^{n-1} \sum_{j=0}^{1} dist_H(B_{ij}, B_{kj}) \\
&\quad + \sum_{\substack{i,k=0 \\ i \neq k}}^{n-1} \sum_{\substack{j,p=0 \\ j \neq p}}^{1} dist_H(B_{ij}, B_{kp}) + \sum_{i=0}^{n-1} \sum_{j=0}^{1} dist_H(B_{ij}, B_{ij}) \Big).
\end{aligned}$$

By Lemma 2.1, we obtain:

$$S_1 = \sum_{i=0}^{n-1} \sum_{\substack{j,p=0 \\ j \neq p}}^{1} dist_H(B_{ij}, B_{ip}) = \sum_{i=0}^{n-1} 6ab = 6abn.$$

Next we compute the sum S_2.

$$\begin{aligned}
S_2 &= \sum_{\substack{i,k=0 \\ i \neq k}}^{n-1} \sum_{j=0}^{1} dist_H(B_{ij}, B_{kj}) \\
&= \sum_{\substack{i,k=0 \\ i \neq k}}^{n-1} \Big(dist_H(B_{i0}, B_{k0}) + dist_H(B_{i1}, B_{k1}) \Big) \\
&= \sum_{\substack{i,k=0 \\ i \neq k \\ v_i v_k \in E(\Lambda)}}^{n-1} \Big(dist_H(B_{i0}, B_{k0}) + dist_H(B_{i1}, B_{k1}) \Big) \\
&\quad + \sum_{\substack{i,k=0 \\ i \neq k \\ v_i v_k \notin E(\Lambda)}}^{n-1} \Big(dist_H(B_{i0}, B_{k0}) + dist_H(B_{i1}, B_{k1}) \Big)
\end{aligned}$$

$$= \sum_{v_iv_k \in E(\Lambda)} \Big(2a^2 + 2b^2\Big) + \sum_{\substack{i,k=0 \\ i \neq k \\ v_iv_k \notin E(\Lambda) \\ dist_\Lambda(v_i,v_k) \text{ is even}}}^{n-1} \Big(dist_H(B_{i0}, B_{k0}) + dist_H(B_{i1}, B_{k1})\Big)$$
$$+ \sum_{\substack{i,k=0 \\ i \neq k \\ v_iv_k \notin E(\Lambda) \\ dist_\Lambda(v_i,v_k) \text{ is odd}}}^{n-1} \Big(dist_H(B_{i0}, B_{k0}) + dist_H(B_{i1}, B_{k1})\Big).$$

By Lemma 2.1, we have

$$S_2 = \sum_{v_iv_k \in E(\Lambda)} \Big(2a^2 + 2b^2\Big) + \sum_{\substack{i,k=0 \\ i \neq k \\ v_iv_k \notin E(\Lambda) \\ dist_\Lambda(v_i,v_k) \text{ is even}}}^{n-1} \Big(a^2 d_G(v_i, v_k) + b^2 d_G(v_i, v_k)\Big)$$
$$+ \sum_{\substack{i,k=0 \\ i \neq k \\ v_iv_k \notin E(\Lambda) \\ dist_\Lambda(v_i,v_k) \text{ is odd}}}^{n-1} \Big(a^2(dist_\Lambda(v_i, v_k) + 1) + b^2(dist_\Lambda(v_i, v_k) + 1)\Big)$$
$$= \Big(\sum_{v_iv_k \in E(\Lambda)} \Big(a^2 + b^2\Big) + \sum_{\substack{i,k=0 \\ i \neq k \\ v_iv_k \notin E(\Lambda)}}^{n-1} (a^2 + b^2) dist_\Lambda(v_i, v_k)\Big) + \sum_{dist_\Lambda(v_i,v_k) \text{ is odd}} (a^2 + b^2).$$

By the definitions of Wiener invariantof Λ and ℓ_1 , we have

$$S_2 = 2\left(a^2 + b^2\right) W(\Lambda) + 2\ell_1 \left(a^2 + b^2\right).$$

Now we compute S_3.

$$S_3 = \sum_{\substack{i,k=0 \\ i \neq k}}^{n-1} \sum_{\substack{j,p=0 \\ j \neq p}}^{1} dist_H(B_{ij}, B_{kp})$$
$$= \sum_{\substack{i,k=0 \\ i \neq k}}^{n-1} \Big(dist_H(B_{i0}, B_{k1}) + dist_H(B_{i1}, B_{k0})\Big)$$

$$= \sum_{\substack{i,k=0 \\ i\neq k \\ dist_\Lambda(v_i,v_k) \text{ is odd}}}^{n-1} \Big(abd_G(v_i,v_k) + abd_G(v_i,v_k)\Big)$$

$$+ \sum_{\substack{i,k=0 \\ i\neq k \\ dist_\Lambda(v_i,v_k) \text{ is even}}}^{n-1} \Big(ab(dist_\Lambda(v_i,v_k)+1) + ab(dist_\Lambda(v_i,v_k)+1)\Big)$$

$$= \sum_{\substack{i,k=0 \\ i\neq k}}^{n-1} 2abd_G(v_i,v_k) + \sum_{dist_\Lambda(v_i,v_k) \text{ is even}} 2ab.$$

By the definitions of $W(\Lambda)$ and ℓ_2 , we have

$$S_3 = 4abW(\Lambda) + 4ab\ell_2.$$

Finally, we compute $S_4 = \sum_{i=0}^{n-1}\sum_{j=0}^{1} dist_H(B_{ij}, B_{ij})$. By Lemma 2.1, we have

$$\begin{aligned} S_4 &= \sum_{i=0}^{n-1}\Big(dist_H(B_{i0},B_{i0}) + dist_H(B_{i1},B_{i1})\Big) \\ &= \sum_{i=0}^{n-1}\Big(2a(a-1) + 2b(b-1)\Big) \\ &= 2n(a^2+b^2-a-b). \end{aligned}$$

Using all the computation above we have:

$$W(H) = (a+b)^2W(\Lambda) + (a^2+b^2)\ell_1 + ab(3n+2\ell_2) + n(a^2+b^2-a-b).$$

□

From the above theorem, we have the following corollaries.

Corollary 2.1. *The Wiener invariant of* $K_n \times K_{a,b}$ *is* $n\Big(n(a^2+b^2+ab)-a-b+2ab\Big)$.

Corollary 2.2. *The Wiener invariant of* $K_n \times K_{a,a}$ *is* $na\Big((3n+2)a-2\Big)$.

3. Reverse Wiener invariant

By using Theorem 2.1 and diameter of Λ, we have following theorem.

Theorem 3.1. *If Λ is a graph on n vertices with each edge of Λ is on a triangle, then*

$$\begin{aligned}\Lambda(\Lambda \times K_{a,b}) =& \frac{n}{2}\Big((n-1)D(\Lambda) - 2(a^2+b^2-a-b+3ab)\Big) \\ & -(a+b)^2 W(\Lambda) - (a^2+b^2)\ell_1 - 2ab\ell_2.\end{aligned}$$

By using above theorem we have the following corollary.

Corollary 3.1. *The reverse Wiener invariant of $K_n \times K_{a,b}$ is*

$$\frac{n}{2}\Big(n(1-2(a^2+b^2+ab)) + 2(a+b-ab) - 1\Big).$$

Corollary 3.2. *The reverse Wiener invariant of $K_n \times K_{a,a}$ is*

$$\frac{n}{2}\Big(n - 2a^2(3n+2) + 4a - 1\Big).$$

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