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The Reliability Wiener Number of Cartesian Product Graphs•

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ABSTRACT Reliability Wiener number is a modification of the original Wiener number in which probabilities are assigned to edges yielding a natural model in which there are some (or all) bonds in the molecule that are not static. Various probabilities naturally allow modelling different types of chemical bonds because chemical bonds are of different types and it is well-known that under certain conditions the bonds can break with certain probability. This is fully taken into account in quantum chemistry. In the model considered here, probabilistic nature is taken into account and at the same time the conceptual simplicity of the discrete graph theoretical model is preserved. Here we extend previous studies by deriving a formula for the reliability Wiener number of a Cartesian product of graphs $G\square H$.

KEYWORDS reliability • Wiener number • Wiener index • Cartesian product of graphs

1. INTRODUCTION

Distance is a basic yet very important notion in many applications of graph theory including mathematical chemistry [2, 3]. The sum of all distances, in mathematical chemistry well known as the Wiener number of a graph [15], is also studied in mathematics [9] and in computer science [8]. Wiener number is the first topological index used in chemical graph theory. Until today, a remarkably large number of modifications and extensions of the Wiener number was put forward (see for example the special issues and books [4, 5]). However, there are relatively few studies of a seemingly natural extension of Wiener number where the meaning of the edge weights are probabilities. The name for the invariant studied here is reliability Wiener number because this generalization of Wiener number was first applied in the context of interconnection networks [12]. We believe that it may be also of interest in chemical graph theory, because the idea to assign probabilities to

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edges is a natural model taking into account that in the structure observed there are some (or all) edges (bonds) that are not static [13]. Various probabilities naturally allow modelling different types of chemical bonds. Namely, chemical bonds are of different types and it is well-known that under certain conditions the bonds can break with certain probability. This is fully taken into account in quantum chemistry. However, a model that would take into account the probabilistic nature and at the same time keep the conceptual simplicity of the discrete graph theoretical model may be a fruitful avenue of research. It was shown in [13] that reliability Wiener number can be used as a measure of branching [10, 11].

Another motivating example is the benzen ring where there are double bonds which form a perfect matching in the complete graph on 6 vertices. There are 10 possible perfect matchings among 6 vertices. Usually, only two matchings that are most probably based on the fixed embedding of the ring into the space are considered (so called Kekulé structures). However it also makes sense to take into account the extended pairings (Dewar, Claus and others) for a given connectivity as was done for example in [1]. Therefore, it may be natural to give certain probabilities to the matchings and thus to double bonds. For example, the two Kekulé structures may naturally be assumed to have probability 1/2 each, but there are other possibilities of course.

Cartesian product of graphs is one of the standard graph products [6]. Well known structures that can be regarded as graph products are meshes and tori that can be obtained as products of paths and cycles, respectively. Wiener number of Cartesian product was studied in [16, 7, 14]. In this paper we show how the reliability Wiener number of a Cartesian product can be computed when knowing the reliability Wiener numbers of factors. In the next section, basic definitions are given. In Section 3, a definition of Cartesian product of edge weighted graph is given and a basic lemma is proved. The main theorem is proved in Section 4.

2. DEFINITIONS

A *weighted graph* $G = (V, E, p)$ is a combinatorial object consisting of an arbitrary set $V = V(G)$ of *vertices*, a set $E = E(G)$ of unordered pairs $\{u, v\} = uv = e$ of distinct vertices of G called *edges*, and a *weighting function*, $p = p_G$. The weight function $p: E(G) \mapsto [0,1]$ is interpreted as the probability of edges. That is, $1 - p(e)$ is the probability that edge $e \in E(G)$ breaks. Hence it is natural to assume that $p(e) > 0$ for any edge of the graph (bond). Alternatively, we can consider the complete graph and model non existing edges by setting $p(e) = 0$. As usual, the order and size of G are denoted by $n = |V(G)|$ and $m = |E(G)|$.

Here, $G \cong H$ denotes graph isomorphism, i.e. the existence of a bijection $b: V(G) \rightarrow V(H)$ such that (1) $g_1,\ g_2$ are connected in G exactly if $b(g_1),\ b(g_2)$ are connected in H and (2) $p_G(g_1, g_2) = p_H(b(g_1), b(g_2))$.

A *path* P between u and v is a sequence of distinct vertices $u = v_0, v_1, v_2, \dots, v_{k-1}, v_k = v$ such that each pair $v_l v_{l+1}$, $(l = i, \dots, k-1)$ is connected by an edge.

We can define the *reliability* of a path P with

$$p(P) = \prod_{l=0}^{k-1} p(v_l, v_{l+1}).$$

In the special case when all edges have probability 1, $p(P) = 1$for any path P.

Of course, several paths from one vertex to another can exist. The maximum reliability between two vertices is reached using the path with maximum reliability. In [12], the notion of *reliability of a graph* was introduced by a version of Wiener number where instead of the usual distance the most reliable path between each pair of vertices is considered. Following this idea, we defined in [13] the reliability Wiener number as follows. For two vertices $u, v \in V(G)$ denote with $P_{\overrightarrow{uv}}$ the set of all directed paths from u to v. The weight of the most reliable path from u to v is called the *reliability of* (u, v):

$$F_{\overrightarrow{uv}} = \max_{P \in P_{\overrightarrow{uv}}} \{p(P)\}. \tag{1}$$

Furthermore, we set $F_{\overrightarrow{uu}} = 1$ for all $u \in V(G)$ and define

$$R^+(u) = \textstyle\sum_{v \in V(G)-u} F_{\overrightarrow{uv}} \text{ the weighted out-reliability of vertex } u,$$
$$R^-(u) = \textstyle\sum_{v \in V(G)-u} F_{\overrightarrow{vu}} \text{ the weighted in-reliability of vertex } u,$$
$$W_{R^+}(G) = \textstyle\sum_{u \in V(G)} R^+(u) \text{ the out-reliability Wiener number of } G,$$
$$W_{R^-}(G) = \textstyle\sum_{u \in V(G)} R^-(u) \text{ the in-reliability Wiener number of } G.$$

As undirected graphs are studied here, obviously, because $p(u, v) = p(v, u) = p(e)$ for any edge $e = \{u, v\}$ in G, $R^-(u) = R^+(u) =: R(u)$ and $W_{R^-}(G) = W_{R^+}(G)$, so we can define the *reliability Wiener number* by

$$W_R(G, p) = \tfrac{1}{2} \textstyle\sum_{u \in V(G)} R(u) = \tfrac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} F_{\overrightarrow{uv}} = \tfrac{1}{2} \sum_{u \neq v} F_{\overrightarrow{uv}}. \tag{2}$$

The reliability Wiener number of G is a measure of the capacity of the vertices of G of transmitting information in a reliable form, where the information is transmitted through the most reliable path. As suggested in [12], the problem of finding $F_{\overrightarrow{uv}}$ can be solved by using Dijkstra's algorithm on a weighted digraph $G' = (V, E, -\ln p)$. Hence W_R can be computed efficiently.

3. THE CARTESIAN PRODUCT OF GRAPHS

First, we generalize the definition of Cartesian product to (edge) weighted Cartesian product of weighted graphs.

Definition 1 *The Cartesian product of weighted graphs G and H is a weighted graph, denoted as $G\square H$, whose vertex set is $V(G\square H) = V(G) \times V(H)$. Two vertices $u = (a, x)$ and $v = (b, y)$ of $G\square H$ are adjacent if $a = b$ and $xy \in E(H)$ or $x = y$ and $ab \in E(G)$. The probabilities (weighting function p) on edges $(u, v) = (a, x)(b, y)$ of a graph $G\square H$ are*

$$p(u,v) = p((a,x)(b,y)) = \begin{cases} p(xy); & if\, a = b and xy \in E(H), \\ p(ab); & if\, x = y and ab \in E(G). \end{cases}$$

Remark. Following the definition of reliability of (1), in the case of undirected Cartesian product of graphs, we will omit arrows and write $F_{(a,x)(b,y)}$.

Lemma 2 *For any two weighted graphs G and H, the reliability of the pair $((a, x), (b, y))$, $F_{(a,x)(b,y)}$, is the product of reliabilities of the projections:*

$$F_{(a,x)(b,y)} = F_{(a,x)(b,x)} \cdot F_{(b,x)(b,y)}. \tag{3}$$

Proof. Let P be arbitrary most reliable path from a to b in G: $a = a_0, a_1, a_2, \ldots, a_n = b$ with the reliability $p(P) = p_0 \cdot p_1 \cdots p_{n-1} = F_{ab}$. Let Q be arbitrary most reliable path from x to y in H: $x = x_0, x_1, x_2, \ldots, x_m = y$ with the reliability $p(Q) = q_0 \cdot q_1 \cdots q_{m-1} = F_{xy}$. This gives rise to two paths in $G\square H$:

$$P \times \{x\} = (a_0, x)(a_1, x)(a_2, x) \cdots (a_n, x)$$

$$\{b\} \times Q = (b, x_0)(b, x_1)(b, x_2) \cdots (b, x_m)$$

with the reliabilities $F_{(a,x)(b,x)} = p(P)$ and $F_{(b,x)(b,y)} = p(Q)$, respectively. Here we use the obvious fact that $F_{(a,x)(b,x)}$ in $G\square H$ is just a copy of F_{ab} in G. The concatenation of these paths is a path from (a, x) to (b, y) with reliability $F_{(a,x)(b,x)} \cdot F_{(b,x)(b,y)}$. Hence, maximizing over all paths from (a, x) to (b, y),

$$F_{(a,x)(b,y)} \geq F_{(a,x)(b,x)} \cdot F_{(b,x)(b,y)}.$$

Conversely, let $\tilde{P}$ be a path from (a, x) and (b, y) in $G\square H$, with maximum reliability. Thus,

$$\tilde{P}: \quad (a,x) = (a_0, x_0)(a_1, x_1)(a_2, x_2) \cdots (a_N, x_N) = (b, y)$$

and

$$F_{(a,x)(b,y)} = p(\tilde{P}) = \tilde{p}_0 \cdot \tilde{p}_1 \cdots \tilde{p}_{N-1}.$$

Using the projections $\Pi_G: G\square H \to G$, $\Pi_G(a,x) = a$and $\Pi_H: G\square H \to H$, $\Pi_H(a,x) = x$ on a path $\tilde{P}$ (for more details see [6]) we find two walks in G and H, respectively:

$$\Pi_G(\tilde{P}):\ a = a_0, a_1, a_2, \dots a_N = b \quad \text{a walk in } G \text{ between } a \text{ and } b,$$
$$\Pi_H(\tilde{P}):\ x = x_0, x_1, x_2, \dots x_N = y \quad \text{a walk in } H \text{ between } x \text{ and } y.$$

From the definition of the product $G\square H$ it is clear that $\Pi_G(a_i x_i) = \Pi_G(a_{i+1}x_{i+1})$ if and only if $\Pi_H(a_i x_i) \neq \Pi_H(a_{i+1}x_{i+1})$, $i = 0,1, \dots N-1$. Denote by $N_G(\tilde{P})$ the set of indices i of vertex-pairs $\Pi_G(a_i x_i), \Pi_G(a_{i+1}x_{i+1})$ for which $\Pi_G(a_i x_i) \neq \Pi_G(a_{i+1}x_{i+1})$, and similarly, $N_H(\tilde{P})$. Obviously, $N_G(\tilde{P})$ and $N_H(\tilde{P})$ are disjoint sets,

$$|N_G(\tilde{P})| + |N_H(\tilde{P})| = N$$

and

$$p(\Pi_G(\tilde{P})) = \prod_{i\in N_G(\tilde{P})} \tilde{p}_i, \qquad p(\Pi_H(\tilde{P})) = \prod_{j\in N_H(\tilde{P})} \tilde{p}_j.$$

Thus,

$$F_{(a,x)(b,y)} = p(\tilde{P}) = p(\Pi_G(\tilde{P})) \cdot p(\Pi_H(\tilde{P})) \leq F_{ab} \cdot F_{xy}.$$

In the last inequality we use the facts that any walk gives rise to a path with reliability that cannot be smaller, and that no path can have greater reliability than most reliable path. Hence reliabilities of projections of $\tilde{P}$ can be bounded from above by F_{ab} and F_{xy}. This completes the proof. □

4. Main Result

Theorem 3 *For any two graphs G and H,*

$$W_R(G\square H) = |G| \cdot W_R(H) + |H| \cdot W_R(G) + 2W_R(G) \cdot W_R(H). \tag{4}$$

Proof. We will divide the sum in the definition (2) of reliability Wiener number for $V(G\square H)$ into three parts: the sum over all pairs where $a = b$, the sum over all pairs where $x = y$ and the sum over all pairs where $a \neq b$ and $x \neq y$.

$$\begin{aligned} W_R(G\square H) &= \tfrac{1}{2}\textstyle\sum_{(a,x),(b,y)\in V(G\square H)} F_{(a,x)(b,y)} \\ &= \tfrac{1}{2}\textstyle\sum_{(a,x),(a,y)\in V(G\square H), x\neq y} F_{(a,x)(b,y)} \\ &\quad + \tfrac{1}{2}\textstyle\sum_{(a,x),(b,x)\in V(G\square H), a\neq b} F_{(a,x)(b,y)} \\ &\quad + \tfrac{1}{2}\textstyle\sum_{(a,x),(b,y)\in V(G\square H), a\neq b, x\neq y} F_{(a,x)(b,y)}. \end{aligned}$$

The first term, using Lemma 2, contributes

$$\frac{1}{2}\sum_{(a,x),(a,y)\in V(G\square H),x\neq y} F_{(a,x)(b,y)} = \frac{1}{2}\sum_{(a,x)(a,y)\in V(G\square H),x\neq y} F_{(a,x)(a,y)} \cdot F_{(a,y)(a,y)}$$

$$= |G| \cdot \frac{1}{2}\sum_{x,y\in V(H),x\neq y} F_{xy}$$

$$= |G| \cdot W_R(H).$$

Analogously, second term gives

$$\frac{1}{2}\sum_{(a,x),(b,x)\in V(G\square H),a\neq b} F_{(a,x)(b,x)} = |H| \cdot W_R(G).$$

In the inner part of the last sum we can use

$$\begin{aligned}\textstyle\sum_{a\in V(G)} \left(\sum_{b\in V(G),b\neq a} F_{(a,x)(a,y)} \cdot F_{(a,y)(b,y)}\right) &= \textstyle\sum_{a\in V(G)} F_{(a,x)(a,y)} \cdot \left(\sum_{b\in V(G),b\neq a} F_{ab}\right)\\ &= \textstyle\sum_{a\in V(G)} F_{(a,x)(a,y)} \cdot R(a)\\ &= F_{xy} \textstyle\sum_{a\in V(G)} R(a)\\ &= 2F_{xy} W_R(G),\end{aligned}$$

where $R(a)$ is the weighted in/out reliability of vertex a, defined in (1). Thus,

$$\frac{1}{2}\sum_{(a,x),(b,y)\in V(G\square H),a\neq b,x\neq y} F_{(a,x)(b,y)} = \frac{1}{2}\sum_{x\in V(H)}\ \sum_{y\in V(H),y\neq x}\ \sum_{a\in V(G)}\ \sum_{b\in V(G),b\neq a} F_{(a,x)(b,y)}$$

$$= \frac{1}{2}\sum_{x\in V(H)} \left(\sum_{y\in V(H),y\neq x} 2F_{xy} W_R(G)\right)$$

$$= W_R(G) \cdot \sum_{x\in V(H)} R(x) = 2W_R(G) \cdot W_R(H).$$

Summing up contributions of the three parts completes the proof. □

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