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Vertex-Weighted Wiener Polynomials for Composite Graphs

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Abstract

Recently introduced vertex-weighted Wiener polynomials are a generalization of both vertex-weighted Wiener numbers and ordinary Wiener polynomials. We present here explicit formulae for vertex-weighted Wiener polynomials of the most frequently encountered classes of composite graphs.

Keywords: Wiener index, Wiener polynomial, Wiener number, composite graph, graph product.

Math. Subj. Class.: 05C12, 05C05, 05C90

1 Introduction

The Wiener number (or Wiener index), first introduced and studied by H. Wiener in 1947 [22], [23], is one of the first, and most important topological indices, i.e. graphic invariants used in the study of structure-property correlations. It has received lots of attention in chemical [17], [14] and also in mathematical literature [15], [3], [7] [25], [24]. Moreover, a fair number of its generalizations and extensions have been introduced and studied, such as the Balaban index [1], the hyper-Wiener index of Randić [16, 12], and Schultz's so-called "molecular topological" index [19]. Many of these generalizations involved suitably chosen vertex-weightings. On the other hand, the fact that the Wiener number can be viewed as the unnormalized first moment of the set of shortest-path distances of a graph, motivated the introduction of higher moments [27, 11, 21, 4] and of the so-called Wiener polynomial ([8] and independently [18]). Sometimes the Wiener polynomial has been called the "Hosoya polynomial", as in references [5]i and [20]. Yet a further extension of the study of Wiener-like graph invariants resulted recently in a unifying approach, achieved by introducing vertex-weighted Wiener polynomials [10].

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The fact that many interesting graphs are composed of simpler graphs, that serve as their basic building blocks, prompted interest in the type of relationship between the Wiener number of a composite graph and Wiener numbers of its building blocks [26]. This development was followed a couple of years later by an article [20] that established corresponding relationships for Wiener polynomials. The main purpose of the present paper is to bring together in a unifying context the line of research of [10] with that of [26] and [20], by giving in an explicit form the formulae for vertex-weighted Wiener polynomials of the most important classes of composite graphs.

The rest of the paper is organized as follows. In section 2 we give the relevant definitions and some preliminary results. In section 3 we state and prove our main results. Finally, those results are illustrated by a few characteristic examples in section 4.

2 Vertex-Weighted Wiener Polynomials

All graphs considered in this paper are simple and connected, unless stated otherwise. For a given graph G we denote by $V(G)$ its vertex set, and by $E(G)$ its edge set. The cardinalities of these two sets are denoted by n and e, respectively, or, if pertaining to a graph G_i, by n_i and e_i, for the corresponding subscript i. The edge $e \in E(G)$ with the endpoints u and v we denote by (u, v). The shortest-path distance between vertices u and v in a graph G is denoted by $D_G(u, v)$, or simply by $D(u, v)$ when there is no possibility of confusion. The degree in G of a vertex $u \in V(G)$ is denoted by $d_G(u)$, or simply by $d(u)$.

The (unweighted) **Wiener polynomial** of G is defined as

$$P_o(G; x) = \sum_{u<v} x^{D(u,v)}$$

with x a dummy variable. This coincides with the definition of Hosoya [8], and Sagan *et al.* [18]. A corresponding (singly) **vertex-weighted** Wiener polynomial is defined

$$P_v(G; x) = \frac{1}{2} \sum_{u<v} [d(u) + d(v)] x^{D(u,v)+1}$$

and a **doubly vertex-weighted** Wiener polynomial is

$$P_{vv}(G; x) = \sum_{u<v} [d(u)d(v)] x^{D(u,v)+2}$$

where $d(u)$ is the degree of vertex u.

The **Wiener number** of a graph G is given by

$$W(G) = \sum_{u<v} D(u, v).$$

The following relationship between the Wiener number and the Wiener polynomial of G was noted in [8], [18]:

$$W(G) = P_0'(G; x)|_{x=1}.$$

The corresponding generalizations for the singly and doubly vertex-weighted cases were given in [10]:

$$W_v(G) = \left[\frac{1}{x} P_v(G; x)\right]'_{x=1}; \quad W_{vv}(G) = \left[\frac{1}{x^2} P_{vv}(G; x)\right]'_{x=1}. \tag{1}$$

Here $W_v(G)$ and $W_{vv}(G)$ denote singly and doubly vertex-weighted Wiener number of G, defined by

$$W_v(G) = \sum_{u<v} \frac{d(u)+d(v)}{2} D(u,v),$$

$$W_{vv}(G) = \sum_{u<v} d(u)d(v)D(u,v),$$

respectively. We refer the reader to the same article for more results on vertex-weighted Wiener polynomials of trees and also of the so-called thorny graphs.

For a vertex $w \in V(G)$ we define the **partial Wiener polynomial** of G with respect to w (or rooted in w):

$$H_0(G;w;x) = \sum_{\substack{u \in V(G) \\ u \neq w}} x^{D(u,w)}.$$

In the same manner, we define singly and doubly vertex-weighted partial Wiener polynomials of G rooted at w:

$$H_v(G;w;x) = \frac{1}{2} \sum_{\substack{u \in V(G) \\ u \neq w}} [d(u)+d(w)] x^{D(u,w)+1};$$

$$H_{vv}(G;w;x) = \sum_{\substack{u \in V(G) \\ u \neq w}} [d(u)d(w)] x^{D(u,w)+2}.$$

The unweighted partial Wiener polynomial was introduced in [20] and independently in [9], and the weighted ones we modelled after [10].

Before we proceed to introduce the composite graphs, let us make the following observation:

Lemma 1. *Let G be a simple, connected, d-regular graph. Then:*

$$P_v(G;x) = dxP_0(G;x);$$

$$P_{vv}(G;x) = d^2x^2P_0(G;x).$$

The proof is obvious from the definitions of P_0, P_v and P_{vv}.

Now we introduce the four standard types of composite graphs that we consider in this paper.

We define the **Cartesian product** $G_1 \times G_2$ as the graph with the vertex set $V(G_1) \times V(G_2)$, with vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ connected by an edge if and only if $[u_1 = v_1$ and $(u_2, v_2) \in E(G_2)]$ or $[u_2 = v_2$ and $(u_1, v_1) \in E(G_1)]$.

Lemma 2. *Let G_1 and G_2 be simple, connected graphs. Then*

$$D_{G_1 \times G_2}(u,v) = D_{G_1}(u_1,v_1) + D_{G_2}(u_2,v_2).$$

The proof is straight-forward but somewhat technical, and we refer the reader to [26], where it is worked out in full detail.

The Cartesian product of G_1 and G_2 is in mathematical literature usually denoted by $G_1 \Box G_2$, but we follow here the notation of Yeh and Gutman [26].

The **sum** of two graphs G_1 and G_2 is defined as a graph $G_1 + G_2$ with the vertex set $V(G_1 + G_2) = V(G_1) \cup V(G_2)$, and the edge set $E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{(u_1, u_2); u_1 \in V(G_1), u_2 \in V(G_2)\}$. In other words, we join every vertex from G_1 to every vertex in G_2. The sum of two graphs is sometimes also called **join**, and denoted by $G_1 \nabla G_2$ ([20]). Obviously, any two vertices of $G_1 + G_2$ are either at the distance 1 or at the distance 2.

The next binary operation we consider is the composition of two graphs. For given graphs G_1 and G_2, their **composition** is the graph $G_1[G_2]$ with the vertex set $V(G_1[G_2]) = V(G_1) \times V(G_2)$, and the vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G_1[G_2]$ are adjacent if and only if $[u_1 = v_1 \in G_1$ and $(u_2, v_2) \in E(G_2)]$, or $[(u_1, v_1) \in E(G_1)]$. In other words, $G_1[G_2]$ is obtained by expanding each vertex of G_1 into a copy of G_2, with each edge of G_1 replaced by the edge set of the corresponding $G_2 + G_2$. The (shortest-path) distance of two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G_1[G_2]$ is given by

$$D_{G_1[G_2]}(u, v) = \begin{cases} D_{G_1}(u_1, v_1) & u_1 \neq v_1; \\ 1 & u_1 = v_1, \quad (u_2, v_2) \in E(G_2); \\ 2 & u_1 = v_1, \quad (u_2, v_2) \notin E(G_2). \end{cases}$$

Finally, for given graphs G_1 and G_2 we define the **cluster** $G_1\{G_2\}$ as the graph obtained by taking one copy of G_1 and $|V(G_1)|$ copies of a rooted graph G_2, and by identifying the root of the i-th copy of G_2 with the i-th vertex of G_1, for $i = 1, \ldots, |V(G_1)|$. We denote the root vertex of G_2 by w, and the copy of G_2 whose root is identified with the vertex $u \in V(G_1)$ by G_2^u. The distance between two vertices $y, z \in G_1\{G_2\}$ is given by

$$D_{G_1\{G_2\}}(y, z) = \begin{cases} D_{G_2}(y, z) & y \in G_2^u, z \in G_2^u; \\ D_{G_1}(u, v) & y = w \in G_2^u, z = w \in G_2^v; \\ D_{G_2}(y, w) + D_{G_1}(u, v) + D_{G_2}(w, z) & y \in G_2^u, z \in G_2^v, u \neq v. \end{cases}$$

There are many more binary operations on graphs, but we restrict our attention to the above four, since their combination and iteration covers most cases of practical interest.

The last part of this preliminary section is concerned with Zagreb indices, a pair of topological indices denoted by $M_1(G)$ and $M_2(G)$ and introduced some 30 years ago [6]. They are defined as follows:

$$M_1(G) = \sum_{u \in V(G)} d(u)^2;$$

$$M_2(G) = \sum_{(u,v) \in E(G)} d(u)d(v).$$

The first Zagreb index can be also expressed as a sum over the edges of G:

$$M_1(G) = \sum_{(u,v) \in E(G)} [d(u) + d(v)].$$

We refer the reader to [13] for the proof of this fact and for more information on Zagreb indices. Obviously, the Zagreb indices can be viewed as the contributions of pairs of adjacent vertices to vertex-weighted Wiener numbers. Curiously enough, it turns out that similar contributions of non-adjacent pairs of vertices must be taken into account when computing vertex-weighted Wiener polynomials of certain composite graphs. Hence we propose to call such contributions Zagreb coindices. More formally, the **first Zagreb coindex** of a graph G is defined by

$$\overline{M}_1(G) = \sum_{(u,v)\notin E(G)} [d(u) + d(v)],$$

and the **second Zagreb coindex** is given by

$$\overline{M}_2(G) = \sum_{(u,v)\notin E(G)} d(u)d(v).$$

The Zagreb indices and Zagreb coindices will be helpful in presenting our main results in a more compact form.

3 Explicit formulae for vertex-weighted Wiener polynomials

In this section we state and prove our main results, by giving explicit formulae for vertex-weighted Wiener polynomials of composite graphs in terms of weighted and unweighted Wiener polynomials and some simple graphic invariants of underlying components. We remind the reader that n_i and e_i denote the respective numbers of vertices and of edges of graph G_i.

Theorem 3. *Let G_1 and G_2 be two simple connected graphs.*

$$\begin{aligned} P_v(G_1 \times G_2; x) = &\\ & 2\left[P_v(G_1; x)P_0(G_2; x) + P_v(G_2; x)P_0(G_1; x)\right] \\ & + n_2 P_v(G_1; x) + 2e_2 x P_0(G_1; x) + n_1 P_v(G_2; x) + 2e_1 x P_0(G_1; x); \end{aligned}$$

$$\begin{aligned} P_{vv}(G_1 \times G_2; x) = &\\ & 2P_{vv}(G_1; x)P_0(G_2; x) + 4P_v(G_1; x)P_v(G_2; x) + 2P_0(G_1; x)P_{vv}(G_2; x) \\ & + n_2 P_{vv}(G_1; x) + 4e_2 x P_v(G_1; x) + M_1(G_2)x^2 P_0(G_1; x) \\ & + n_1 P_{vv}(G_2; x) + 4e_1 x P_v(G_2; x) + M_1(G_1)x^2 P_0(G_2; x). \end{aligned}$$

Proof. It is obvious from the definition of $G_1 \times G_2$ that

$$d_{G_1 \times G_2}(u_1, u_2) = d_{G_1}(u_1) + d_{G_2}(u_2).$$

Though in this proof we allow the arguments of various distances and degrees to specify the relevant graphs, so that this becomes $d(u_1, u_2) = d(u_1) + d(u_2)$. Then rephrasing the definition of $P_v(G; x)$ as $\frac{1}{4}\sum_{u\neq v}[d_G(u) + d_G(v)]x^{D_G(u,v)+1}$, we chose $G = G_1 \times G_2$ and further make use of Lemma 2 to obtain

$$
\begin{aligned}
&P_v(G_1 \times G_2; x) \\
&\quad = \frac{1}{4} \sum_{u_1 \neq v_1} \sum_{u_2 \neq v_2} [d(u_1) + d(u_2) + d(v_1) + d(v_2)]\, x^{D(u_1,v_1)} x^{D(u_2,v_2)} x \\
&\qquad + \frac{1}{4} \sum_{u_1 \neq v_1} \sum_{u_2 = v_2} [d(u_1) + d(v_1) + 2d(u_2)]\, x^{D(u_1,v_1)+1} \\
&\qquad + \frac{1}{4} \sum_{u_2 \neq v_2} \sum_{u_1 = v_1} [d(u_2) + d(v_2) + 2d(u_1)]\, x^{D(u_2,v_2)+1} \\
&\quad = \frac{1}{4} \sum_{u_1 \neq v_1} \Bigg[[d(u_1) + d(v_1)]\, x^{D(u_1,v_1)+1} \sum_{u_2 \neq v_2} x^{D(u_2,v_2)} \\
&\qquad\quad + x^{D(u_1,v_1)} \sum_{u_2 \neq v_2} [d(u_2) + d(v_2)]\, x^{D(u_2,v_2)+1} \Bigg] \\
&\qquad + \frac{1}{4} \sum_{u_2 = v_2} \left[\sum_{u_1 \neq v_1} [d(u_1) + d(v_1)]\, x^{D(u_1,v_1)+1} + [d(u_2) + d(v_2)]\, x \sum_{u_1 \neq v_1} x^{D(u_1,v_1)} \right] \\
&\qquad + \frac{1}{4} \sum_{u_1 = v_1} \left[\sum_{u_2 \neq v_2} [d(u_2) + d(v_2)]\, x^{D(u_2,v_2)+1} + [d(u_1) + d(v_1)]\, x \sum_{u_2 \neq v_2} x^{D(u_2,v_2)} \right] \\
&\quad = \frac{1}{4} \sum_{u_1 \neq v_1} \left[2P_0(G_2; x)\, [d(u_1) + d(v_1)]\, x^{D(u_1,v_1)+1} + 4P_v(G_2; x) x^{D(u_1,v_1)} \right] \\
&\qquad + \frac{1}{4} \sum_{u_2 = v_2} [4P_v(G_1; x) + 2xP_0(G_1; x) \cdot 2d(u_2)] \\
&\qquad + \frac{1}{4} \sum_{u_1 = v_1} [4P_v(G_2; x) + 2xP_0(G_2; x) \cdot 2d(u_1)] \\
&\quad = 2P_v(G_1; x)P_0(G_2; x) + 2P_v(G_2; x)P_0(G_1; x) \\
&\qquad + n_2 P_v(G_1; x) + 2e_2 x P_0(G_1; x) + n_1 P_v(G_2; x) + 2e_1 x P_0(G_2; x).
\end{aligned}
$$

To achieve the last equality we have used the fact that $\sum_{u \in V(G)} d(u) = 2e$, for a general graph G. And the first result of the theorem is attained.

In order to prove our second claim, we start from the rephrased definition of $P_{vv}(G; x)$ as $\frac{1}{2} \sum_{u \neq v} d_G(u) d_G(v) x^{D_G(u,v)+2}$ and take $G = G_1 \times G_2$.

$$
P_{vv}(G_1 \times G_2; x) = \frac{1}{2} \sum_{u \neq v} [d(u_1) + d(v_1)]\, [d(u_2) + d(v_2)]\, x^{D(u_1,v_1)+D(u_2,v_2)+2}.
$$

Again, the sum can be split into three sums,

$$
\frac{1}{2} \sum_{u_1 \neq v_1} \sum_{u_2 \neq v_2}, \quad \frac{1}{2} \sum_{u_1 = v_1} \sum_{u_2 \neq v_2}, \quad \text{and} \quad \frac{1}{2} \sum_{u_2 = v_2} \sum_{u_1 \neq v_1},
$$

which we respectively denote by S_1, S_2, and S_3. Now we have:

$$\begin{aligned}
S_1 = \frac{1}{2}\sum_{u_1\neq v_1}\Bigg[& d(u_1)d(u_2)x^{D(u_1,v_1)+2}\sum_{u_2\neq v_2} x^{D(u_2,v_2)} \\
& + d(u_1)x^{D(u_1,v_1)+1}\sum_{u_2\neq v_2} d(v_2)x^{D(u_2,v_2)+1} \\
& + d(v_1)x^{D(u_1,v_1)+1}\sum_{u_2\neq v_2} d(u_2)x^{D(u_2,v_2)+1} \\
& + x^{D(u_1,v_1)}\sum_{u_2\neq v_2} d(u_2)d(v_2)x^{D(u_2,v_2)+2}\Bigg] \\
= 2P_{vv}(G_1;x)P_0(G_2;x) & + 4P_v(G_1;x)P_v(G_2;x) + 2P_0(G_1;x)P_{vv}(G_2;x),
\end{aligned}$$

where $\sum_{u\neq v} d(u)x^{D(u,v))+1} = 2P_v(G;x)$ has been used.

Next

$$\begin{aligned}
S_2 = {} & \frac{1}{2}\sum_{u_1=v_1} d(u_1)^2 \sum_{u_2\neq v_2} x^{D(u_2,v_2)} \\
& + \frac{1}{2}\sum_{u_1=v_1} d(u_1)x\left[\sum_{u_2\neq v_2} d(v_2)x^{D(u_2,v_2)+1} + \sum_{u_2\neq v_2} d(u_2)x^{D(u_2,v_2)+1}\right] \\
& + \frac{1}{2}\sum_{u_1=v_1} x^{D(u_1,v_1)}\sum_{u_2\neq v_2} d(u_2)d(v_2)x^{D(u_2,v_2)+2} \\
= {} & x^2P_0(G2;x)\sum_{u_1} d(u_1)^2 + xP_v(G_2);x)\sum_{u_1} d(u_1) + P_{vv}(G_2;x)\sum_{u_1} 1 \\
= {} & M_1(G_1)x^2P_0(G_2;x) + 4e_1xP_v(G_2;x) + n_1P_{vv}(G_2;x).
\end{aligned}$$

Now because of the symmetry between S_2 and S_3, one obtains S_3 by switching the roles of G_1 and G_2 in S_2. Addition of S_1, S_2, and S_3 yields the second result of the theorem. □

Theorem 4. *Let G_1 and G_2 be two simple graphs.*

$$\begin{aligned}
P_v(G_1+G_2;x) = {} & \left[\frac{1}{2}\left[\overline{M}_1(G_1)+\overline{M}_1(G_2)\right] + n_2\left[\binom{n_1}{2} - e_1\right] + n_1\left[\binom{n_2}{2} - e_2\right]\right]x^3 \\
& + \left[\frac{1}{2}\left[M_1(G_1)+M_1(G_2)\right] + 2(e_1n_2+n_1e_2) + \frac{1}{2}n_1n_2(n_1+n_2)\right]x^2;
\end{aligned}$$

$$\begin{aligned}
& P_{vv}(G_1+G_2;x) = \\
& \Bigg[\overline{M}_2(G_1)+\overline{M}_2(G_2)+n_2\overline{M}_1(G_1)+n_1\overline{M}_1(G_2)+n_1^2\left[\binom{n_2}{2}-e_2\right]+ \\
& n_2^2\left[\binom{n_1}{2}-e_1\right]\Bigg]x^4 + \Big[M_2(G_1)+M_2(G_2)+n_2M_1(G_1)+n_1M_1(G_2)+ \\
& n_1^2n_2^2+3e_1n_2^2+3e_2n_1^2+4e_1e_2\Big]x^3.
\end{aligned}$$

Proof. As already observed, all vertices of $G_1 + G_2$ are either at distance 1, or at distance 2. The vertices at distance 2 are precisely those of G_1 that are not adjacent in G_1, and those of G_2 that are not adjacent in G_2. Furthermore, for a vertex $u \in V(G_1)$ we have $d_{G_1+G_2}(u) = d_{G_1}(u) + n_2$, and for a vertex $v \in V(G_2)$, we have $d_{G_1+G_2}(v) = d_{G_2}(v) + n_1$. Hence, we can conclude that $P_v(G_1 + G_2; x) = a_3x^3 + a_2x^2$, and $P_{vv}(G_1 + G_2; x) = b_4x^4 + b_3x^3$. The coefficients a_2, a_3, b_3, and b_4 can be determined by a straightforward computation. For example,

$$\begin{aligned} a_3 &= \frac{1}{2} \sum_{\substack{u<v \\ (u,v)\notin E(G_1)}}^{\in G_1} [d(u) + d(v) + 2n_2] + \frac{1}{2} \sum_{\substack{u<v \\ (u,v)\notin E(G_2)}}^{\in G_2} [d(u) + d(v) + 2n_1] \\ &= \frac{1}{2} \sum_{e\notin E(G_1)} [d(u) + d(v)] + \frac{1}{2} \sum_{e\notin E(G_2)} [d(u) + d(v)] + n_2 \left|E(\overline{G}_1)\right| + n_1 \left|E(\overline{G}_2)\right| \\ &= \frac{1}{2} \left[\overline{M}_1(G_1) + \overline{M}_1(G_2)\right] + n_2 \left[\binom{n_1}{2} - e_1\right] + n_1 \left[\binom{n_2}{2} - e_2\right]. \end{aligned}$$

Similarly,

$$\begin{aligned} a_2 &= \frac{1}{2} \sum_{\substack{u<v \\ (u,v)\in E(G_1)}} [d(u) + d(v) + 2n_2] + \frac{1}{2} \sum_{\substack{u<v \\ (u,v)\in E(G_2)}} [d(u) + d(v) + 2n_1] \\ &\quad + \frac{1}{2} \sum_{u\in G_1} \sum_{v\in G_2} [d(u) + d(v) + n_1 + n_2] \\ &= \frac{1}{2} M_1(G_1) + n_2e_1 + \frac{1}{2} M_1(G_2) + n_1e_2 + \frac{1}{2} \sum_{u\in G_1} \left[d(u)n_2 + n_2^2 + n_1n_2 + 2e_2\right] \\ &= \frac{1}{2} [M_1(G_1) + M_1(G_2)] + 2(e_1n_2 + n_1e_2) + \frac{1}{2} n_1n_2(n_1 + n_2). \end{aligned}$$

The coefficients b_4 and b_3 can be determined in a completely analogous manner, though we omit the details. □

Theorem 5. *Let G_1 and G_2 be simple graphs, and let G_1 be connected. Then:*

$$\begin{aligned} P_v(G_1[G_2]; x) = n_2^3 P_v(G_1; x) &+ 2n_2e_2xP_0(G_1; x) \\ &+ \left[\frac{n_1}{2} M_1(G_2) + 2e_1e_2n_2\right] x^2 \\ &+ \left[\frac{n_1}{2} \overline{M}_1(G_2) + 2e_1n_2 \left[\binom{n_2}{2} - e_2\right]\right] x^3; \end{aligned}$$

$$\begin{aligned} P_{vv}(G_1[G_2]; x) = n_2^4 P_{vv}(G_1; x) &+ 4e_2n_2^2xP_v(G_1; x) + 4e_2^2x^2P_0(G_1; x) \\ &+ \left[n_1M_2(G_2) + 2e_1n_2M_1(G_2) + e_2n_2^2M_1(G_1)\right] x^3 \\ &+ \left[n_1\overline{M}_2(G_2) + 2e_1n_2\overline{M}_1(G_2) + n_2^2 \left[\binom{n_2}{2} - e_2\right] M_1(G_1)\right] x^4. \end{aligned}$$

Proof. We start from the observation

$$d_{G_1[G_2]}(u_1, u_2) = d_{G_2}(u_2) + n_2d_{G_1}(u_1).$$

Taking into account our formula for distance in $G_1[G_2]$, given immediately after the definition of composition of two graphs, we have the following:

$$\begin{aligned}
&P_v(G_1[G_2];x)\\
&\quad= \frac{1}{4}\sum_{u\neq v}\left[d(u)+d(v)\right]x^{D(u,v)+1}\\
&\quad= \frac{1}{4}\sum_{u_2}\sum_{v_2}\Bigg[\left[d(u_2)+d(v_2)\right]x\sum_{u_1\neq v_1}x^{D(u_1,v_1)+1}\\
&\qquad\qquad + n_2\sum_{u_1\neq v_1}\left[d(u_1)+d(v_1)\right]x^{D(u_1,v_1)+1}\Bigg]\\
&\qquad + \frac{1}{2}\sum_{u_1=v_1}\left[\sum_{e\in E(G_2)}\left[d(u_2)+d(v_2)\right]+n_2\left[d(u_1)+d(v_1)\right]\sum_{e\in E(G_2)}1\right]x^2\\
&\qquad + \frac{1}{2}\sum_{u_2=v_2}\left[\sum_{e\notin E(G_2)}\left[d(u_2)+d(v_2)\right]+n_2\left[d(u_1)+d(v_1)\right]\sum_{e\notin E(G_2)}1\right]x^3\\
&\quad= \frac{1}{4}\left[2xP_0(G_1;x)\sum_{u_2}\sum_{v_2}\left[d(u_2)+d(v_2)\right]+4n_2P_v(G_1;x)\sum_{u_2}\sum_{v_2}1\right]\\
&\qquad + \frac{1}{2}\sum_{u_1=v_1}\left[M_1(G_2)+e_2n_2\left[d(u_1)+d(v_1)\right]\right]x^2\\
&\qquad + \frac{1}{2}\left[\sum_{u_1=v_1}\overline{M}_1(G_2)+n_2|E(\bar(G)_2)|\sum_{u_1=v_1}\left[d(u_1)+d(v_1)\right]\right]x^3\\
&\quad= n_2^3P_v(G_1;x)+2n_2e_2xP_0(G_1;x)\\
&\qquad + \left[\frac{n_1}{2}M_1(G_2)+2e_1e_2n_2\right]x^2\\
&\qquad + \left[\frac{n_1}{2}\overline{M}_1(G_2)+2e_1n_2\left[\binom{n_2}{2}-e_2\right]\right]x^3;
\end{aligned}$$

The expression for $P_{vv}(G_1[G_2];x)$ is obtained in much the same manner, and we omit the details. □

Theorem 6. *Let G_1 and G_2 be simple connected graphs. Let the copies of G_2 used in the construction of $G_1\{G_2\}$ be rooted in vertex w, and let $d_{G_2}(w)=t$. Then:*

$$\begin{aligned}
&P_v(G_1\{G_2\};x) =\\
&\quad \left[H_0(G_2;w;x)+1\right]P_v(G_1;x)+n_1P_v(G_2;x)\\
&\qquad + \Big[H_0(G_2;w;x)\left[2H_v(G_2;w;x)-txH_0(G_2;w;x)\right]\\
&\qquad\qquad + 2H_v(G_2;w;x)+tx\Big]P_0(G_1;x)+e_1xH_0(G_2;w;x);
\end{aligned}$$

$$\begin{aligned}
&P_{vv}(G_1\{G_2\};x) =\\
&\quad P_{vv}(G_1;x)+n_1P_{vv}(G_2;x)
\end{aligned}$$

$$+ 2\left[2H_v(G_2;w;x) - txH_0(G_2;w;x) + tx\right] P_v(G_1;x)$$
$$+ \left[2H_{vv}(G_2;w;x) + \left[2H_v(G_2;w;x) - txH_0(G_2;w;x)\right]^2 + t^2x^2\right] P_0(G_1;x)$$
$$+ 2e_1x\left[2H_v(G_2;w;x) - txH_0(G_2;w;x)\right].$$

Proof. Here we follow the "fivefold path" employed in [10]. We partition our sum in five sums as follows.

The first sum S_1 consists of contributions to $P_v(G_1\{G_2\};x)$ of pairs of vertices from G_1. For a vertex $u \in V(G_1)$, we have

$$d_{G_1\{G_2\}}(u) = d_{G_1}(u) + t,$$

since u serves as an anchor-point for a copy of G_2, and the root vertex of this copy has degree t. Taking this into account, we obtain

$$\begin{aligned} S_1 &= \frac{1}{2}\sum_{u<v}^{\in G_1}\left[d(u)+d(v)\right]x^{D(u,v)+1} \\ &= \frac{1}{2}\sum_{u<v}^{\in G_1}\left[d_{G_1}(u)+d_{G_1}(v)\right]x^{D(u,v)+1} + \frac{1}{2}\cdot 2tx\sum_{u<v}^{\in G_1}x^{D(u,v)} \\ &= P_v(G_1;x) + txP_0(G_1;x). \end{aligned}$$

The second sum S_2 is taken over all pairs of vertices such that one of them, u, is in G_1, and the other one is in G_2^u, the copy of G_2 that is anchored at u. Thence

$$\begin{aligned} S_2 &= \frac{1}{2}\sum_{u\in G_1}\sum_{\substack{v\in G_2^u\\ v\neq u}}\left[d_{G_1}(u)+d_{G_1}(v)\right]x^{D(u,v)+1} \\ &= \frac{1}{2}\sum_{u\in G_1}\sum_{\substack{v\in G_2^u\\ v\neq u}} d_{G_1}(u)x^{D(u,v)+1} + \frac{1}{2}\sum_{u\in G_1}\sum_{\substack{v\in G_2^u\\ v\neq u}}\left[d_{G_2}(v)+t\right]x^{D(u,v)+1} \\ &= e_1xH_0(G_2;w;x) + n_1H_v(G_2;w;x). \end{aligned}$$

The third sum S_3 is over all pairs of vertices such that one of them, u, is in G_1, and the other one is in some G_2^z, where $z \neq u$.

$$\begin{aligned} S_3 &= \frac{1}{4}\sum_{u\in G_1}\sum_{\substack{v\in G_2^z\\ z\neq u}}\left[d(u)+d(v)\right]x^{D(u,v)+1} \\ &= \frac{1}{4}\sum_{u\in G_1}\sum_{z\in G_1}\sum_{v\in G_2^z}\left[d_{G_1}(u)+t+d(v)\right]x^{D(u,z)+D(z,v)+1} \\ &\quad + \frac{1}{4}\sum_{z\in G_1}\sum_{u\in G_1}\sum_{v\in G_2^u}\left[d_{G_1}(z)+t+d(v)\right]x^{D(u,z)+D(z,v)+1} \\ &= \frac{1}{4}H_0(G_2;w;x)\sum_{u\in G_1}\sum_{z\in G_1}\left[d_{G_1}(u)+d_{G_1}(z)\right]x^{D(u,z)+1} \\ &\quad + \frac{1}{4}\cdot 2H_v(G_2;w;x)\left[\sum_{u\in G_1}\sum_{z\in G_1}x^{D(u,z)} + \sum_{z\in G_1}\sum_{u\in G_1}x^{D(z,u)}\right] \end{aligned}$$

$$= H_0(G_2; w; x)P_v(G_1; x) + 2H_v(G_2; w; x)P_0(G_1; x).$$

The fourth sum S_4 is taken over all pairs of non-root vertices in G_2^u, and then over all $u \in G_1$.

$$\begin{aligned}
S_4 &= \frac{1}{2} \sum_{u \in G_1} \sum_{\substack{v<z \\ v \neq u, z \neq u}}^{\in G_2} \left[d_{G_2}(v) + d_{G_2}(z)\right] x^{D(v,z)+1} \\
&= \frac{1}{2} \sum_{u \in G_1} \left[2P_v(G_2; x) - 2H_v(G_2; w; x)\right] \\
&= n_1 P_v(G_2; x) - n_1 H_v(G_2; w; x).
\end{aligned}$$

Finally, the fifth sum S_5 is over all pairs of non-root vertices from different copies of G_2. For such a pair $v \in G_2^u$, $z \in G_2^y$, we have

$$D(v, z) = D_{G_2}(v, u) + D_{G_1}(u, y) + D_{G_2}(y, z) = D_{G_2}(v, w) + D_{G_1}(u, y) + D_{G_2}(w, z).$$

Now,

$$\begin{aligned}
S_5 &= \frac{1}{4} \sum_{u \in G_1} \sum_{y \in G_1} \sum_{v \in G_2^u} \sum_{z \in G_2^y} \left[d(v) + d(z)\right] x^{D(v,z)+1} \\
&= \frac{1}{4} \sum_{u \in G_1} \sum_{y \in G_1} \sum_{v \in G_2^u} \sum_{z \in G_2^y} \left[d_{G_2}(v) + d_{G_2}(z) + 2t - 2t\right] x^{D(v,u)} x^{D(u,y)} x^{D(y,z)} x \\
&= \frac{1}{4} \sum_{u \in G_1} \sum_{y \in G_1} [H_0(G_2; w; x) x^{D(u,y)} \sum_{v \in G_2^u} \left[t + d_{G_2}(v)\right] x^{D(v,u)+1} \\
&\quad - 2txx^{D(u,y)} H_0(G_2; w; x) \sum_{v \in G_2^u} x^{D(v,u)} \\
&\quad + 2H_v(G_2; w; x) x^{D(u,y)} \sum_{v \in G_2^u} x^{D(v,u)}] \\
&= \frac{1}{4} \left[4H_0(G_2; w; x)H_v(G_2; w; x) - 2txH_0(G_2; w; x)^2\right] \sum_{u \in G_1} \sum_{y \in G_1} x^{D(u,y)} \\
&= H_0(G_2; w; x) \left[2H_v(G_2; w; x) - txH_0(G_2; w; x)\right] P_0(G_1; x).
\end{aligned}$$

The formula for $P_v(G_1\{G_2\}; x)$ follows upon addition of the quantities S_1, S_2, S$_3$, S_4, and S_5.

The formula for $P_{vv}(G_1\{G_2\}; x)$ follows in much the same way. □

4 Corrolaries and examples

In this section our theorems for vertex-weighted Wiener polynomials are illustrated for several more particular composite graphs.

Let P_n and C_n denote the path and the cycle on n vertices, respectively. It is well known, and it can be easily checked, that their unweighted Wiener polynomials are given by the expressions:

$$P_0(P_n; x) = \sum_{k=1}^{n-1} (n - k)x^k;$$

$$P_0(C_n;x) = n \sum_{k=1}^{\lfloor n/2 \rfloor -1} x^k + a_n x^{\lfloor n/2 \rfloor},$$

where $a_n = \frac{n}{2}$ for n even, and $a_n = n$ for n odd. Singly and doubly vertex-weighted Wiener polynomials of P_n are given by

$$P_v(P_n;x) = (x+1)P_0(P_n;x) - (n-1)x$$

and

$$P_{vv}(P_n;x) = (x+1)^2 P_0(P_n;x) - (3n-4)x^2 - (n-1)x,$$

respectively. This follows from results given in [10] that give weighted Wiener polynomials of trees in terms of unweighted ones.

The expressions for the vertex-weighted Wiener polynomials of the $m \times n$ **rectangular grid** follow as this is the Cartesian product graph $P_m \times P_n$.

Corollary 7.

$$\begin{aligned} &P_v(P_m \times P_n;x) = \\ &\quad (x+1)\left[4P_0(P_m;x)P_0(P_n;x) + nP_0(P_m;x) + mP_0(P_n;x)\right] - (2mn-m-n)x; \\ &P_{vv}(P_m \times P_n;x) = \\ &\quad 8(x+1)^2 P_0(P_m;x)P_0(P_n;x) + \left[(2-n)x^2 + 2x + n\right] P_0(P_m;x) \\ &\qquad + \left[(2-m)x^2 + 2x + m\right] P_0(P_n;x) + 2(4m+4n-5mn-2)x^2 \\ &\qquad - (2mn-m-n)x. \end{aligned}$$

For $m = n$, one has the square grid:

Corollary 8.

$$\begin{aligned} P_v(P_n \times P_n;x) &= 4(x+1)P_0(P_n;x)^2 + 2n(x+1)P_0(P_n;x) - 2n(n-1)x; \\ P_{vv}(P_n \times P_n;x) &= 8(x+1)^2 P_0(P_n;x)^2 + 2[(2-n)x^2 + 2x + n]P_0(P_n;x) \\ &\quad - 2(5n^2 - 8n + 2)x^2 - 2n(n-1)x. \end{aligned}$$

For $m = 2$, one has the **ladder graph** on n rungs, L_n.

Corollary 9.

$$\begin{aligned} P_v(L_n;x) &= 2(x+1)(2x+1)P_0(P_n;x) - 2(n-1)x; \\ P_{vv}(L_n;x) &= 2(x+1)(2x+1)^2 P_0(P_n;x) - (n-2)x^3 - 2(6n-7)x^2 - 2(n-1)x. \end{aligned}$$

It follows from Lemma 1 that the vertex-weighted Wiener polynomials of C_n are given by

$$\begin{aligned} P_v(C_n;x) &= 2xP_0(C_n;x); \\ P_{vv}(C_n;x) &= 4x^2 P_0(C_n;x). \end{aligned}$$

Using this fact and Theorem 3, we can compute vertex-weighted Wiener polynomials of a **cylinder graph** $P_m \times C_n$.

Corollary 10.

$$\begin{aligned} P_v(P_m \times C_n; x) &= 2(3x+1)P_0(P_m; x)P_0(C_n; x) + n(3x+2)P_0(P_m; x) \\ &\quad + 2mxP_0(C_n; x) - n(m-1)x; \\ P_{vv}(P_m \times C_n; x) &= 2(3x+1)^2 P_0(P_m; x)P_0(C_n; x) + n(3x+1)^2 P_0(P_m; x) \\ &\quad + 2[(m+1)x^2 - m + 1]P_0(C_n; x) + n(8-7m)x^2 - n(m-1)x. \end{aligned}$$

For $m = 2$ in Corrolary 10, vertex-weighted Wiener polynomials of an n sided **prism**, Pr_n, result:

Corollary 11.

$$\begin{aligned} P_v(Pr_n; x) &= 6x(x+1)P_0(C_n; x) + 3nx^2; \\ P_{vv}(Pr_n; x) &= 18x^2(x+1)P_0(C_n; x) + 9nx^3. \end{aligned}$$

Corrolary 11 could have also been obtained by first computing $P_0(Pr_n; x)$ via theorem 1 of reference [20], and then using 3-regularity of Pr_n and applying Lemma 1. The same approach gives us expressions for vertex-weighted Wiener polynomials of a (4-regular) **torus graph** $C_m \times C_n$.

Corollary 12.

$$\begin{aligned} P_v(C_m \times C_n; x) &= 4x[2P_0(C_m; x)P_0(C_n; x) + nP_0(C_m; x) + mP_0(C_n; x)]; \\ P_{vv}(C_m \times C_n; x) &= 16x^2[2P_0(C_m; x)P_0(C_n; x) + nP_0(C_m; x) + mP_0(C_n; x)]. \end{aligned}$$

Next, we give vertex-weighted Wiener polynomials for the **fence graph** $P_n[K_2]$.

Corollary 13.

$$\begin{aligned} P_v(P_n[K_2]; x) &= 4(3x+2)P_0(P_n; x) + (5n-4)x^2 - 8(n-1)x; \\ P_{vv}(P_n[K_2]; x) &= 4(3x+2)^2 P_0(P_n; x) + (25n-32)x^3 - 16(4n-5)x^2 - 16(n-1)x. \end{aligned}$$

For a **closed fence**, $C_n[K_2]$, we get the following:

Corollary 14.

$$\begin{aligned} P_v(C_n[K_2]; x) &= 20xP_0(C_n; x) + 5x^2; \\ P_{vv}(C_n[K_2]; x) &= 100x^2 P_0(C_n; x) + 25x^3. \end{aligned}$$

The result can be obtained either from Theorem 5, of by combining Theorem A and Lemma 1.

Our last example is concerned with t-fold **bristled graph** of P_n. (For a given graph G, its t-fold bristled graph is obtained by attaching t vertices of degree 1 to each vertex of G.) This graph can be represented as the cluster of P_n and the t-star graph $K_{1,t}$.

Corollary 15.

$$\begin{aligned} P_v(P_n\{K_{1,t}\}; x) &= (x+1)(tx+1)^2 P_0(P_n; x) \\ &\quad + n\binom{t}{2}x^3 + n\binom{t+1}{2}x^2 - (n-1)x; \\ P_{vv}(P_n\{K_{1,t}\}; x) &= (x+1)^2(tx+1)^2 P_0(P_n; x) + n\binom{t}{2}x^4 \\ &\quad + nt^2x^3 - [2t(n-1) + 3n - 4]x^2 - (n-1)x. \end{aligned}$$

The result follows by a straightforward application of Theorem 6, taking $K_{1,t}$ to be rooted in its mid-vertex w, and taking into account the following formulae for its partial Wiener polynomials:

$$H_0(K_{1,t}; w; x) = tx; \quad H_v(K_{1,t}; w; x) = \binom{t+1}{2} x^2; \quad H_{vv}(K_{1,t}; w; x) = t^2 x^3.$$

The t-fold bristled graph of a cycle on n vertices, $C_n\{K_{1,t}\}$, is the same object as the $(t-2)$-thorny graph of the n-cycle [10], and it can be easily checked that the formulae for $P_v(C_n\{K_{1,t}\}; x)$ and $P_{vv}(C_n\{K_{1,t}\}; x)$ coincide with those given in [10] for this thorny graph.

We conclude by pointing out that the vertex-weighted Wiener numbers of the considered composite graphs can now be easily computed by using formulae (1). For example, from (1) and Corrolary 12 it follows at once that

$$\begin{aligned}
&W_v(C_m \times C_n)\\
&= 4\frac{d}{dx}\left[2P_0(C_m; x)P_0(C_n; x) + nP_0(C_m; x) + mP_0(C_n; x)\right]_{x=1}\\
&= 8\left[P_0(C_m; x)P_0'(C_n; x)\right]_{x=1} + 8\left[P_0'(C_m; x)P_0(C_n; x)\right]_{x=1} + 4nW(C_m) + 4mW(C_n)\\
&= 8\binom{m}{2} W(C_n) + 8\binom{n}{2} W(C_m) + 4nW(C_m) + 4mW(C_n)\\
&= 4[n^2 W(C_m) + m^2 W(C_n)].
\end{aligned}$$

The Wiener number of the n-cycle is $\frac{1}{8}n^3$ for n even, and $\frac{1}{8}(n^3 - n)$ for n odd [2]. Taking both n and m even in the above example yields

$$W_v(C_m \times C_n) = \frac{1}{2} m^2 n^2 (m+n).$$

The given theorems might be specialized to yet further special pairs of graphs.

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