

RESEARCH ARTICLE

On the Wiener Polarity Index of Lattice Networks

Lin Chen¹, Tao Li^{2*}, Jinfeng Liu¹, Yongtang Shi¹, Hua Wang³

1 Center for Combinatorics and LPMC-TJKLC, Nankai University, Tianjin, China, **2** College of Computer and Control Engineering, Nankai University, Tianjin 300071, China, **3** Department of Mathematical Sciences Georgia Southern University, Statesboro, GA 30460-8093, United States of America

* litao@nankai.edu.cn



CrossMark
click for updates

OPEN ACCESS

Citation: Chen L, Li T, Liu J, Shi Y, Wang H (2016) On the Wiener Polarity Index of Lattice Networks. PLoS ONE 11(12): e0167075. doi:10.1371/journal.pone.0167075

Editor: Cheng-Yi Xia, Tianjin University of Technology, CHINA

Received: August 25, 2016

Accepted: November 8, 2016

Published: December 8, 2016

Copyright: © 2016 Chen et al. This is an open access article distributed under the terms of the [Creative Commons Attribution License](https://creativecommons.org/licenses/by/4.0/), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

Data Availability Statement: There is no data in this paper.

Funding: This work was supported by The National Science Foundation of China (No. 11371021), Recipient: Yongtang Shi; The Natural Science Foundation of Tianjin (No. 16JCYBJC15200), Recipient: Tao Li; and The Simons Foundation (No. 245307), Recipient: Hua Wang. The funders had no role in study design, data collection and analysis, decision to publish, or preparation of the manuscript.

Competing Interests: The authors have declared that no competing interests exist.

Abstract

Network structures are everywhere, including but not limited to applications in biological, physical and social sciences, information technology, and optimization. Network robustness is of crucial importance in all such applications. Research on this topic relies on finding a suitable measure and use this measure to quantify network robustness. A number of distance-based graph invariants, also known as topological indices, have recently been incorporated as descriptors of complex networks. Among them the Wiener type indices are the most well known and commonly used such descriptors. As one of the fundamental variants of the original Wiener index, the Wiener polarity index has been introduced for a long time and known to be related to the cluster coefficient of networks. In this paper, we consider the value of the Wiener polarity index of lattice networks, a common network structure known for its simplicity and symmetric structure. We first present a simple general formula for computing the Wiener polarity index of any graph. Using this formula, together with the symmetric and recursive topology of lattice networks, we provide explicit formulas of the Wiener polarity index of the square lattices, the hexagonal lattices, the triangular lattices, and the $3^3 \cdot 4^2$ lattices. We also comment on potential future research topics.

Introduction

Robustness is the ability of a network to maintain performance when encountering attacks or enduring partial failure. In order to decide whether a given network is robust, a way to quantitatively measure network robustness is needed. Once such a measure has been established, it can serve as a standard for comparing networks or a guidance for improving existing networks and designing new networks. Intuitively robustness is all about back-up possibilities, or alternative paths, but it is rather challenging to capture all these concepts in a simple mathematical formula. During the recent years a lot of robustness measures have been proposed by scientists from different backgrounds, including but not limited to Biology, Chemistry, Computer Science, Engineering, Physics, and Mathematics [1–7]. Generally a network is considered as a graph consisting of a set of vertices connected by edges, and the study of network robustness relies on the analysis of such underlying graphs.

One way to measure a network structure is through the so called structure descriptors, or topological indices [8]. In theoretical biology and chemistry, for instance, molecular structure descriptors are numerical parameters mathematically derived from the graph structure. They have been found to be useful for modeling physico-chemical, toxicologic, pharmacologic, biological and other properties of molecular compounds. These descriptors are mainly divided into three types: degree-based indices, distance-based indices and spectrum-based indices. Degree-based indices contain the (general) Randić index [9–11], the (general) zeroth order Randić index [12, 13], the Zagreb index [14, 15], the connective eccentricity index [16] and so on [17]. Distance-based indices [18] include the Balaban index [19, 20], the Wiener index and Wiener polarity index [21], the Kirchhoff index [22, 23] and so forth. Eigenvalues of graphs [24], various of graph energies [25–36], the HOMO-LUMO index [37, 38], and the Estrada index [39–41] belong to spectrum-based indices. There are also some topological indices defined based on both degrees and distances, such as the degree distance [42] and graph entropies [43, 44]. The study of mathematical properties of such graph indices and the evaluation of them in various graph structures have been of tremendous interest to researchers.

A *lattice graph*, or simply a *lattice*, is a graph possessing a drawing whose embedding in a Euclidean space \mathbb{R}^n forms a regular tiling. Because of the symmetric nature of its topology, lattice graphs appear to be among the most common network structures. For exactly the same reason, the computation of various physical and chemical indices of various lattice graphs has attracted the attention of many scientists as well as mathematicians. See, for instance, [45–51]. We will focus on the square lattices, the hexagonal lattices, the triangular lattices, and the $3^3 \cdot 4^2$ lattices, each corresponding to a grid with specific geometric shapes.

In this paper all graphs under consideration are finite, connected, undirected and simple. For standard notations and terminologies we follow [52]. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The *distance* $d_G(u, v)$ (or simply $d(u, v)$ when there is no confusion) between two vertices u and v of G is the length of the shortest path that connects u and v . One of the most well-known and well-studied distance-based graph indices is the *Wiener number* $W(G)$, also termed as *Wiener index* in chemical or mathematical chemistry literatures. It is defined as the sum of distances over all unordered vertex pairs in G [21]. I.e.,

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

As a representative of successful structure-descriptors, the Wiener index has received much attention. For further details we refer the readers to some recent papers [53–56] and the comprehensive survey of Dobrynin, Entringer and Gutman [57].

Another important molecular descriptor was also introduced by Wiener [21], called the *Wiener polarity index*. Denoted by $W_p(G)$, it is defined as the number of unordered pairs of vertices that are at distance 3 in G . That is,

$$W_p(G) = |\{(u, v) | d_G(u, v) = 3, u, v \in V(G)\}|. \quad (1)$$

In organic compounds, say paraffin, the Wiener polarity index is the number of pairs of carbon atoms which are separated by three carbon-carbon bonds. Based on the Wiener index and the Wiener polarity index, the formula

$$t_B = aW(G) + bW_p(G) + c,$$

was used to calculate the boiling points t_B of the paraffins, where a , b and c are constants for a given isomeric group.

In an acyclic structure, the Wiener polarity index can be expressed in terms of vertex degrees (see, for instance, Lemma 2). This unique characteristic of the Wiener polarity index makes it interesting for studies from both distance-based and degree-based points of view. However, compared with the Wiener index, surprisingly little attention has been paid to the Wiener polarity index until very recently. Nevertheless, the study of the Wiener polarity index has indeed caught the attention of many researchers. By using the Wiener polarity index, Lukovits and Linert demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons in [58]. Hosoya in [59] found a physical-chemical interpretation of $W_p(G)$. Du et al. [60] described a linear time algorithm for computing the Wiener polarity index of trees and characterized the trees maximizing the index among all the trees of the given order. Later, Deng, Xiao and Tang characterized the extremal trees with respect to this index among all trees of order n and diameter k [61]. While for cycle-containing graphs, the maximum Wiener polarity index of unicyclic graphs and the corresponding extremal graphs were determined in [62]. In [63] Ma et al. determined the sharp upper bound of the Wiener polarity index among all bicyclic networks based on some graph transformations. Moreover, the extremal values of catacondensed hexagonal systems, hexagonal cacti and polyphenylene chains with respect to the Wiener polarity index were computed in [64]. It was proved that the Wiener polarity index of fullerenes with n carbon atoms is $(9n - 60)/2$ in the same paper. Recently, Hua and Das [65] established an upper bound on the Wiener polarity index in terms of Hosoya index and characterized the corresponding extremal graphs. They also obtained Nordhaus-Gaddum-type results for $W_p(G)$. Other recent work on Wiener polarity index can be found in [66–70].

In this paper we study the Wiener polarity index of several common classes of lattices. In the section of Preliminaries and the square lattices, we first introduce some notations and previously established fundamental results on the Wiener polarity index of graphs. Through the concept of 3rd neighborhoods, we provide a simple but extremely useful formula for calculating the Wiener polarity index. We also present the computation of the Wiener polarity index of square lattices as an example of applications of such results. In the sections that follow, we discuss in details the computation of the Wiener polarity index of the hexagonal lattices, the triangular lattices, and the $3^3 \cdot 4^2$ lattices. We summarize our findings and propose some future directions of research in the section of Concluding remarks.

Preliminaries and the square lattices

In this section, we first recall some notations. Then a general formula is presented for the Wiener polarity index of any graph. In mathematics, a *Cartesian product* is a mathematical operation which returns a product set (or simply product) from multiple sets. Given sets A and B , the Cartesian product of A and B , generally denoted by $A \square B$, is the set of all ordered pairs (a, b) , where $a \in A$ and $b \in B$. That is,

$$A \square B = \{(a, b) | a \in A, b \in B\}.$$

Given graphs G and H with vertex sets U and V , the *Cartesian product* $G \square H$ of graphs G and H is a graph such that the vertex set of $G \square H$ is $U \square V$, and any two vertices (u, u') and (v, v') are adjacent in $G \square H$ if and only if either $u = v$ and u' is adjacent to v' in H , or $u' = v'$ and u is adjacent to v in G .

For a graph G and vertex $v \in V(G)$, let $N_G(v)$ denote the neighborhood of v and $d_G(v) = |N_G(v)|$ denote the degree of v . The greatest distance between any two vertices in G is the diameter of G , denoted by $diam(G)$. The girth $g(G)$ of G , is the length of a shortest cycle in G . For any integer i , we call $N_G^i(v) = \{u \in V(G) | d_G(u, v) = i\}$ the *i th neighborhood* of v , and the

vertices in $N_G^i(v)$ are called the *ith neighbors* of v . In particular, $N_G^1(v)$ is precisely the neighborhood $N_G(v)$ of v , $N_G^0(v) = \{v\}$, while $N_G^i(v) = \emptyset$ for $i > \text{diam}(G)$. In addition, let P_n and C_n denote the path and the cycle with n vertices, respectively.

The following lemmas are useful in the study of the Wiener polarity index of the lattice networks.

Lemma 1 ([69]) *Let G and H be two non-trivial connected graphs, then*

$$W_p(G \square H) = W_p(G)|V(H)| + W_p(H)|V(G)| + 2W_2(G)m(H) + 2W_2(H)m(G),$$

where $m(G)$ and $m(H)$ are the number of edges of G and H , respectively, and $W_2(G) = |\{\{u, v\} | d_G(u, v) = 2, u, v \in V(G)\}|$ is the number of unordered pairs of vertices $\{u, v\}$ of G such that $d_G(u, v) = 2$.

Lemma 2 ([60]) *Let $T = (V, E)$ be a tree. Then*

$$W_p(T) = \sum_{uv \in E} (d_T(u) - 1)(d_T(v) - 1).$$

Lemma 3 ([62, 67]) *Let $U = (V, E)$ be a unicyclic graph. Let C denote the unique cycle of U :*

- *If $g(U) = 3$ with $V(C) = \{v_1, v_2, v_3\}$, then*

$$W_p(U) = \sum_{uv \in E} (d_U(u) - 1)(d_U(v) - 1) + 9 - 2d_U(v_1) - 2d_U(v_2) - 2d_U(v_3);$$

- *If $g(U) = 4$ with $V(C) = \{v_1, v_2, v_3, v_4\}$, then*

$$W_p(U) = \sum_{uv \in E} (d_U(u) - 1)(d_U(v) - 1) + 4 - d_U(v_1) - d_U(v_2) - d_U(v_3) - d_U(v_4);$$

- *If $g(U) \geq 5$, then*

$$W_p(U) = \begin{cases} \sum_{uv \in E} (d_U(u) - 1)(d_U(v) - 1) - 5, & \text{if } g(U) = 5, \\ \sum_{uv \in E} (d_U(u) - 1)(d_U(v) - 1) - 3, & \text{if } g(U) = 6, \\ \sum_{uv \in E} (d_U(u) - 1)(d_U(v) - 1), & \text{if } g(U) \geq 7. \end{cases}$$

Lastly, we provide a simple general formula for the Wiener polarity index of a graph, which plays an important role in the proofs of our main results.

Lemma 4 *For any graph G , the Wiener polarity index $W_p(G)$ of G can be expressed as*

$$W_p(G) = \frac{\sum_{v \in V(G)} |N_G^3(v)|}{2}. \tag{2}$$

Proof. By the definitions of the Wiener polarity index and the *ith* neighborhood, we have

$$W_p(G) = |\{(u, v) | d_G(u, v) = 3, u, v \in V(G)\}|$$

and

$$|N_G^3(v)| = |\{(u, v) | d_G(u, v) = 3, u \in V(G)\}|.$$

Formula (2) then follows immediately.

To study the Wiener polarity index of lattice networks, we first consider the simple case concerning the square lattices.

Let $P_m \square P_n (m \geq 2, n \geq 2)$, $P_m \square C_n (m \geq 2, n \geq 3)$, and $C_m \square C_n (m \geq 3, n \geq 3)$ denote the square lattices with free, cylindrical and toroidal boundary conditions respectively, it is easy to see that $P_m \square P_n$ is a sequence of spanning subgraphs of the sequence $P_m \square C_n$ of finite graphs, and $P_m \square C_n$ is a sequence of spanning subgraphs of the sequence $C_m \square C_n$ of finite graphs. Following the aforementioned lemmas, the Wiener polarity index of the square lattices can be easily calculated. In the rest of this section, we assume without loss of generality, that $n \geq m$ in $P_m \square P_n$ and $C_m \square C_n$.

Theorem 1 Let $P_m \square P_n$, $P_m \square C_n$ and $C_m \square C_n$ denote the square lattices with free, cylindrical and toroidal boundary conditions, respectively. Then

$$W_p(P_m \square P_n) = \begin{cases} 4n - 10, & \text{if } m = 2, n \geq 3; \\ 6mn - 9m - 9n + 8, & \text{if } m \geq 3, n \geq 3; \end{cases} \tag{3}$$

$$W_p(P_m \square C_n) = \begin{cases} 4n, & \text{if } m = 2, n \geq 7; \\ 9m - 21, & \text{if } m \geq 3, n = 3; \\ 16m - 32, & \text{if } m \geq 3, n = 4; \\ 25m - 45, & \text{if } m \geq 3, n = 5; \\ 33m - 54, & \text{if } m \geq 3, n = 6; \\ 6mn - 9n, & \text{if } m \geq 3, n \geq 7; \end{cases} \tag{4}$$

$$W_p(C_m \square C_n) = \begin{cases} 9n, & \text{if } m = 3, n \geq 7; \\ 16n, & \text{if } m = 4, n \geq 7; \\ 25n, & \text{if } m = 5, n \geq 7; \\ 33n, & \text{if } m = 6, n \geq 7; \\ 6mn, & \text{if } m \geq 7, n \geq 7. \end{cases} \tag{5}$$

Proof. It follows from Lemma 2 that $W_p(P_2) = 0$ and $W_p(P_m) = m - 3$ for $m \geq 3$. On the other hand, Lemma 3 yields that $W_p(C_3) = W_p(C_4) = W_p(C_5) = 0$, $W_p(C_6) = 3$, and $W_p(C_n) = n$ for $n \geq 7$. By the definition of $W_2(G)$, it is not difficult to see that $W_2(P_m) = m - 2$ for $m \geq 2$, $W_2(C_3) = 0$, $W_2(C_4) = 2$, and $W_2(C_n) = n$ for $n \geq 5$. In addition, by Lemma 1 we have

$$\begin{aligned} W_p(P_m \square P_n) &= W_p(P_m)|V(P_n)| + W_p(P_n)|V(P_m)| + 2W_2(P_m)m(P_n) \\ &\quad + 2W_2(P_n)m(P_m), \end{aligned}$$

proving Eq (3).

Similarly, Eqs (4) and (5) are also direct consequences of Lemma 1 and the above discussion.

Remark 1 For small values of m and n , still by Lemma 1, we have the followings:

$$W_p(P_2 \square P_2) = 0; W_p(P_2 \square C_3) = 0, W_p(P_2 \square C_4) = 4, W_p(P_2 \square C_5) = 10, W_p(P_2 \square C_6) = 18;$$

$$W_p(C_3 \square C_3) = 0, W_p(C_3 \square C_4) = 12, W_p(C_3 \square C_5) = 30, W_p(C_3 \square C_6) = 45, W_p(C_4 \square C_4) = 32,$$

$$W_p(C_4 \square C_5) = 60, W_p(C_4 \square C_6) = 84, W_p(C_5 \square C_5) = 100, W_p(C_5 \square C_6) = 135, W_p(C_6 \square C_6) = 180.$$

The Wiener polarity index of the hexagonal lattices

Next we consider the Wiener polarity index of the hexagonal lattices. We follow the notations in [50]. The hexagonal lattices with toroidal, cylindrical and free boundary conditions, are denoted by $H^t(n, m)$, $H^c(n, m)$ and $H^f(n, m)$, respectively, where $(a_1, b_1), (a_2, b_2), \dots, (a_{m+1}, b_{m+1}); (a_1, c_1^*), (c_1, c_2^*), (c_2, c_3^*), \dots, (c_{n-1}, c_n^*), (c_n, b_{m+1})$ are edges in $H^t(n, m)$ (as illustrated in Fig 1). The hexagonal lattice $H^c(n, m)$ is obtained from $H^t(n, m)$ by deleting edges $(a_1, c_1^*), (c_1, c_2^*), (c_2, c_3^*), \dots, (c_{n-1}, c_n^*), (c_n, b_{m+1})$. If the edges $(a_1, b_1), (a_2, b_2), \dots, (a_{m+1}, b_{m+1})$ are also removed, then the hexagonal lattice $H^f(n, m)$ with free boundary condition is obtained. It is easy to see that $|V(H^t(n, m))| = |V(H^c(n, m))| = |V(H^f(n, m))| = 2(n + 1)(m + 1)$. Furthermore, from the definitions it is obvious that $H^f(n, m)$ and $H^c(n, m)$ are spanning subgraphs of $H^t(n, m)$. In the following result we assume, without loss of generality, that $m \geq n$ in $H^t(n, m)$ and $H^f(n, m)$.

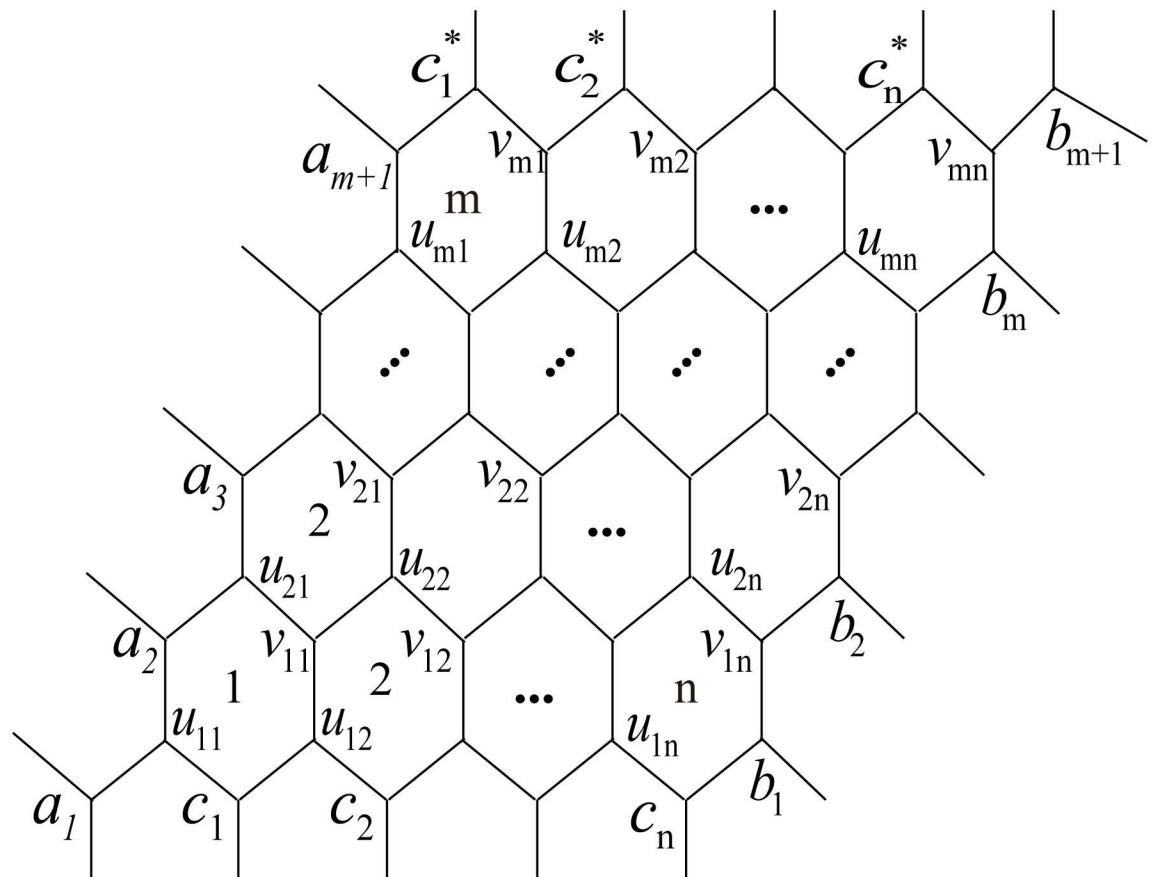


Fig 1. The hexagonal lattice.

doi:10.1371/journal.pone.0167075.g001

Theorem 2 For the hexagonal lattices $H^t(n, m)$, $H^c(n, m)$ and $H^f(n, m)$ with toroidal, cylindrical and free boundary conditions, we have

$$W_p(H^t(n, m)) = \begin{cases} 10(m + 1), & \text{if } n = 1, m \geq 3; \\ 24(m + 1), & \text{if } n = 2, m \geq 3; \\ 9(n + 1)(m + 1), & \text{if } n \geq 3, m \geq 3; \end{cases}$$

$$W_p(H^c(n, m)) = \begin{cases} 10m - 4, & \text{if } n = 1, m \geq 1; \\ 24m - 3, & \text{if } n = 2, m \geq 1; \\ 9m(n + 1), & \text{if } n \geq 3, m \geq 1; \end{cases}$$

$$W_p(H^f(n, m)) = 9nm - 2 \quad \text{for } n \geq 1, m \geq 1.$$

Remark 2 As illustrated in Fig 2, we generally have

$$W_p(H^t(n, m)) > W_p(H^c(n, m)) > W_p(H^f(n, m)),$$

with the common asymptotic value $9mn$ as both m and n approaches infinity.

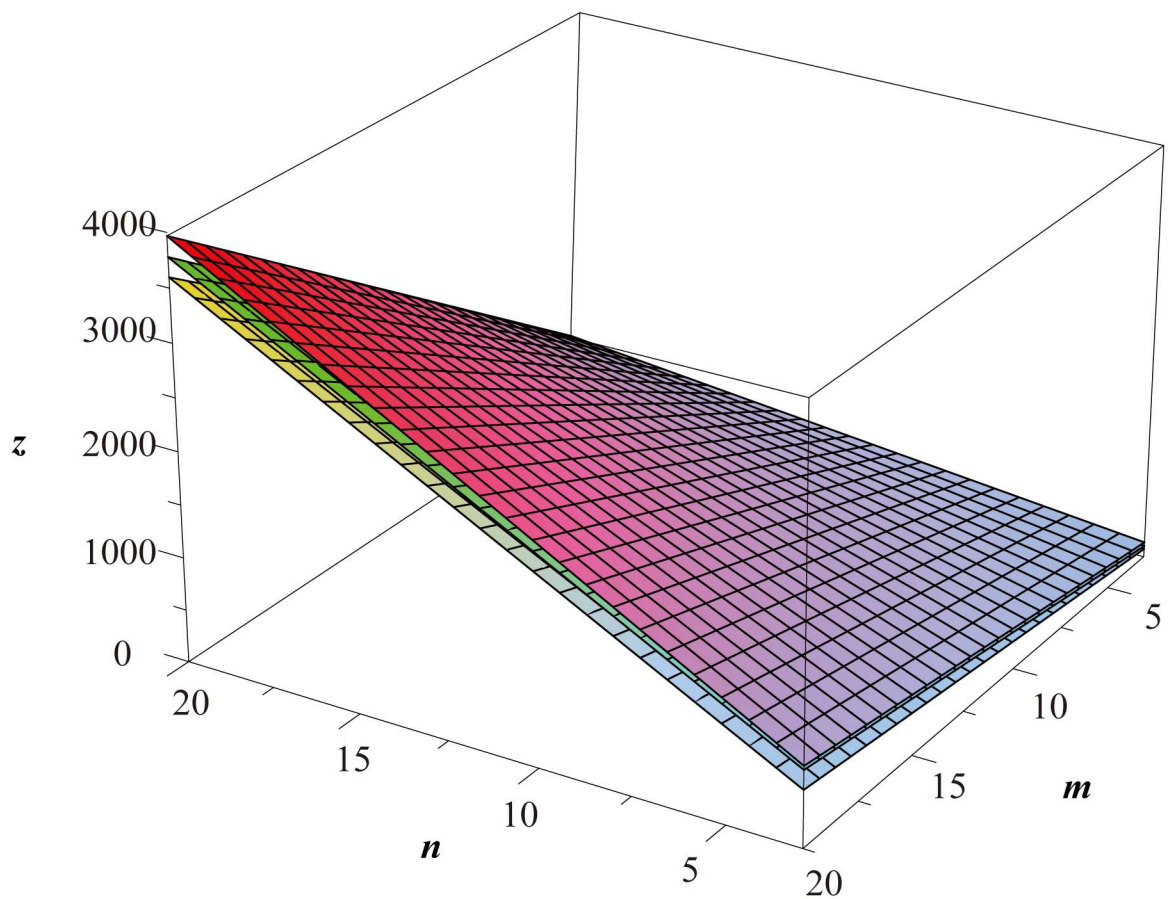


Fig 2. The Wiener polarity index of $H^t(n, m)$, $H^c(n, m)$ and $H^f(n, m)$.

doi:10.1371/journal.pone.0167075.g002

Proof. We consider each of these three lattices through different cases.

(1) First consider $H^t(n, m)$. Our argument relies on the simple fact that every vertex in $H^t(n, m)$ has the same number of 3rd neighbors. Take, for instance, vertex a_1 from Fig 1:

- If $n = 1$ and $m \geq 3$, then

$$N_{H^t(1,m)}^3(a_1) = \{u_{21}, b_2, u_{m1}, b_m, b_{m+1}\}.$$

Hence the number of 3rd neighbors of any vertex in $H^t(1, m)$ is 5 and Lemma 4 implies that

$$W_p(H^t(1, m)) = \frac{\sum_{v \in H^t(1,m)} |N_{H^t(1,m)}^3(v)|}{2} = \frac{5 \times 2(1+1)(m+1)}{2} = 10(m+1).$$

- If $n = 2$ and $m \geq 3$, then

$$N_{H^t(2,m)}^3(a_1) = \{u_{21}, b_2, u_{12}, c_2^*, b_{m+1}, u_{22}, u_{m1}, u_{m2}\}.$$

Thus the number of 3rd neighbors of any vertex in $H^t(2, m)$ is 8 and Lemma 4 implies that

$$W_p(H^t(2, m)) = \frac{\sum_{v \in H^t(2,m)} |N_{H^t(2,m)}^3(v)|}{2} = \frac{8 \times 2(2+1)(m+1)}{2} = 24(m+1).$$

- If $n \geq 3$ and $m \geq 3$, then

$$N_{H^t(n,m)}^3(a_1) = \{u_{21}, b_2, u_{12}, c_2^*, u_{1n}, b_{m+1}, u_{2n}, u_{m1}, u_{m2}\}.$$

Similarly we have

$$\begin{aligned} W_p(H^t(n, m)) &= \frac{\sum_{v \in H^t(n,m)} |N_{H^t(n,m)}^3(v)|}{2} = \frac{9 \times 2(n+1)(m+1)}{2} \\ &= 9(n+1)(m+1). \end{aligned}$$

(2) In the case of $H^c(n, m)$ (Fig 1), we can make similar observations on vertices whose 3rd neighborhood share the same cardinality. For this purpose we partition the vertex set $H^c(n, m)$ into $m + 1$ disjoint classes:

•

$$V_0 = \{a_1, c_1, c_2, \dots, c_n, c_1^*, c_2^*, \dots, c_n^*, b_{m+1}\},$$

•

$$V_1 = \{u_{11}, u_{12}, \dots, u_{1n}, b_1, a_{m+1}, v_{m1}, v_{m2}, \dots, v_{mn}\},$$

•

$$V_2 = \{a_2, v_{11}, v_{12}, \dots, v_{1n}, u_{m1}, u_{m2}, \dots, u_{mn}, b_m\},$$

⋮

•

$$V_m = \{u_{(\frac{m+1}{2})1}, u_{(\frac{m+1}{2})2}, \dots, u_{(\frac{m+1}{2})n}, b_{\frac{m+1}{2}}, a_{(\frac{m+1}{2})+1}, v_{(\frac{m+1}{2})1}, v_{(\frac{m+1}{2})2}, \dots, v_{(\frac{m+1}{2})n}\}$$

when m is odd, or

$$V_m = \{a_{\frac{m}{2}+1}, v_{\frac{m}{2}1}, v_{\frac{m}{2}2}, \dots, v_{\frac{m}{2}n}, u_{(\frac{m}{2}+1)1}, u_{(\frac{m}{2}+1)2}, \dots, u_{(\frac{m}{2}+1)n}, b_{\frac{m}{2}+1}\}$$

when m is even.

Since vertices in the same class have the same number of 3rd neighbors, we only need to consider one vertex from each class.

- If $n = 1$, it is easy to see that $W_p(H^c(1, 1)) = 6$ and $W_p(H^c(1, 2)) = 16$. When $m \geq 3$, one can verify the followings:

$$N_{H^c(1,m)}^3(a_1) = \{u_{21}, b_2\}, \quad N_{H^c(1,m)}^3(u_{11}) = \{a_3, v_{11}, v_{21}\},$$

$$N_{H^c(1,m)}^3(a_2) = \{u_{31}, b_3, b_1\}, \quad N_{H^c(1,m)}^3(u_{21}) = \{a_1, c_1, v_{21}, a_4, v_{31}\},$$

$$N_{H^c(1,m)}^3(a_i) = \{u_{(i-2)1}, b_{i-1}, b_{i-2}, u_{(i+1)1}, b_{i+1}\} \left(3 \leq i \leq \lfloor \frac{m}{2} \rfloor + 1\right),$$

$$N_{H^c(1,m)}^3(u_{i1}) = \{a_{i-1}, v_{(i-2)1}, v_{i1}, v_{(i+1)1}, a_{i+2}\} \left(3 \leq i \leq \lfloor \frac{m}{2} \rfloor\right).$$

That is, $|N_{H^c(1,m)}^3(v)| = 2$ for $v \in V_0$, $|N_{H^c(1,m)}^3(v)| = 3$ for $v \in V_1$ or $v \in V_2$, and $|N_{H^c(1,m)}^3(v)| = 5$ for any vertex v in $V' = V(H^c(1, m)) - V_0 - V_1 - V_2$. By Lemma 4,

$$\begin{aligned} W_p(H^c(1, m)) &= \frac{\sum_{v \in V(H^c(1,m))} |N_{H^c(1,m)}^3(v)|}{2} \\ &= \frac{2 \times |V_0| + 3 \times |V_1| + 3 \times |V_2| + 5 \times |V'|}{2} \\ &= \frac{2 \times 4 + 3 \times 4 + 3 \times 4 + 5 \times [4(m+1) - 4 \times 3]}{2} \\ &= 10m - 4. \end{aligned}$$

It is not hard to check that $W_p(H^c(1, 1))$ (with $m = 1$) and $W_p(H^c(1, 2))$ (with $m = 2$) also satisfy this expression.

- If $n = 2$, then $W_p(H^c(2, 1)) = 21$ and $W_p(H^c(2, 2)) = 45$. When $m \geq 3$, the 3rd neighborhoods of the representative vertices are

$$N_{H^c(2,m)}^3(a_1) = \{u_{21}, b_2, u_{12}, u_{22}\},$$

$$N_{H^c(2,m)}^3(u_{11}) = \{a_3, v_{11}, v_{12}, v_{22}, c_2\},$$

$$N_{H^c(2,m)}^3(a_2) = \{u_{31}, b_3, u_{12}, u_{22}, b_1, u_{32}\},$$

$$N_{H^c(2,m)}^3(u_{21}) = \{a_1, c_1, v_{12}, v_{22}, c_2, v_{21}, a_4, v_{32}\},$$

$$N_{H^c(2,m)}^3(a_i) = \{u_{(i-2)1}, b_{i-1}, u_{(i-2)2}, u_{(i-1)2}, u_{i2}, u_{(i+1)2}, b_{i+1}, u_{(i+1)1}\}$$

for $3 \leq i \leq \lfloor \frac{m}{2} \rfloor + 1$, and

$$N_{H^c(2,m)}^3(u_{i1}) = \{a_{i-1}, v_{(i-2)1}, v_{(i-1)2}, v_{i2}, v_{(i-2)2}, v_{i1}, v_{(i+1)2}, a_{i+2}\}$$

for $3 \leq i \leq \lceil \frac{m}{2} \rceil$.

Hence $|N_{H^c(2,m)}^3(v)| = 4$ for $v \in V_0$, $|N_{H^c(2,m)}^3(v)| = 5$ for $v \in V_1$, $|N_{H^c(2,m)}^3(v)| = 6$ for $v \in V_2$, and $|N_{H^c(2,m)}^3(v)| = 8$ for any vertex v in $V' = V(H^c(2, m)) - V_0 - V_1 - V_2$. Consequently

$$\begin{aligned} W_p(H^c(2, m)) &= \frac{\sum_{v \in V(H^c(2,m))} |N_{H^c(2,m)}^3(v)|}{2} \\ &= \frac{4 \times |V_0| + 5 \times |V_1| + 6 \times |V_2| + 8 \times |V'|}{2} \\ &= \frac{4 \times 6 + 5 \times 6 + 6 \times 6 + 8 \times [6(m+1) - 6 \times 3]}{2} \\ &= 24m - 3, \end{aligned}$$

which also holds for $m = 1$ and $m = 2$.

- If $n \geq 3$, we have, for $m = 1$ or $m = 2$,

$$W_p(H^c(n, 1)) = 9(n + 1)$$

and

$$W_p(H^c(n, 2)) = 18(n + 1).$$

When $m \geq 3$, similar to before we have

$$|N_{H^c(n,m)}^3(v)| = 5 \quad \text{for } v \in V_0,$$

$$|N_{H^c(n,m)}^3(v)| = 6 \quad \text{for } v \in V_1,$$

$$|N_{H^c(n,m)}^3(v)| = 7 \quad \text{for } v \in V_2,$$

and

$$|N_{H^c(n,m)}^3(v)| = 9 \quad \text{for } v \in V' = V(H^c(n, m)) - V_0 - V_1 - V_2.$$

Hence

$$\begin{aligned} W_p(H^c(n, m)) &= \frac{\sum_{v \in V(H^c(n,m))} |N_{H^c(n,m)}^3(v)|}{2} \\ &= \frac{5 \times |V_0| + 6 \times |V_1| + 7 \times |V_2| + 9 \times |V'|}{2} \\ &= \frac{5(2n + 2) + 6(2n + 2) + 7(2n + 2) + 9(2n + 2)(m - 2)}{2} \\ &= 9m(n + 1), \end{aligned}$$

also satisfied by $W_p(H^c(n, 1))$ and $W_p(H^c(n, 2))$.

(3) Lastly, we will evaluate the Wiener polarity index of $H^f(n, m)$ recursively.

First consider the case $n = 1$. Through direct computation we have, in $H^f(1, m)$, the followings when $m \geq 3$:

$$\begin{aligned} |N_{H^f(1,m)}^3(a_1)| &= |N_{H^f(1,m)}^3(b_{m+1})| = 2, \\ |N_{H^f(1,m)}^3(u_{11})| &= |N_{H^f(1,m)}^3(v_{m1})| = 2, \\ |N_{H^f(1,m)}^3(a_2)| &= |N_{H^f(1,m)}^3(b_m)| = 3, \\ |N_{H^f(1,m)}^3(u_{i1})| &= |N_{H^f(1,m)}^3(v_{(m+1-i)1})| = 4 \text{ for } 2 \leq i \leq m-1, \\ |N_{H^f(1,m)}^3(a_i)| &= |N_{H^f(1,m)}^3(b_{m+2-i})| = 5 \text{ for } 3 \leq i \leq m, \\ |N_{H^f(1,m)}^3(u_{m1})| &= |N_{H^f(1,m)}^3(v_{11})| = 3, \\ |N_{H^f(1,m)}^3(a_{m+1})| &= |N_{H^f(1,m)}^3(b_1)| = 4, \text{ and} \\ |N_{H^f(1,m)}^3(c_1^*)| &= |N_{H^f(1,m)}^3(c_1)| = 2. \end{aligned}$$

Thus

$$\begin{aligned} W_p(H^f(1, m)) &= \frac{\sum_{v \in V(H^f(1,m))} |N_{H^f(1,m)}^3(v)|}{2} \\ &= \frac{[2 + 2 + 3 + 4(m-2) + 5(m-2) + 3 + 4 + 2] \times 2}{2} \\ &= 9m - 2, \end{aligned}$$

also satisfied by $W_p(H^f(1, 1)) = 7$ and $W_p(H^f(1, 2)) = 16$.

Now let $n \geq 2$. The structure of $H^f(n, m)$ yields

$$\begin{aligned} W_p(H^f(n, m)) &= |\{(u, v) | d_{H^f(n,m)}(u, v) = 3, u, v \in V(H^f(n, m))\}| \\ &= |N_{H^f(n,m)}^3(a_1)| + |N_{H^f(n,m)}^3(u_{11})| + |N_{H^f(n,m)}^3(a_2)| \\ &\quad + \sum_{i=2}^m (|N_{H^f(n,m)}^3(u_{i1})| - 1) + \sum_{i=3}^{m+1} (|N_{H^f(n,m)}^3(a_i)| - 1) \\ &\quad + (|N_{H^f(n,m)}^3(c_1^*)| - 1) + W_p(H^f(n-1, m)). \end{aligned}$$

Here $(|N_{H^f(n,m)}^3(u_{i1})| - 1)$ and $(|N_{H^f(n,m)}^3(a_i)| - 1)$ appear because of the double counted terms.

By applying this recursion we can explicitly compute $W_p(H^f(n, m))$ for $n \geq 2$.

For $m \geq 3$, it is not difficult to check the 3rd neighborhoods individual vertices, we skip the details. As a result we have

$$\begin{aligned} &|N_{H^f(n,m)}^3(a_1)| + |N_{H^f(n,m)}^3(u_{11})| + |N_{H^f(n,m)}^3(a_2)| + \sum_{i=2}^m (|N_{H^f(n,m)}^3(u_{i1})| - 1) \\ &+ \sum_{i=3}^{m+1} (|N_{H^f(n,m)}^3(a_i)| - 1) + (|N_{H^f(n,m)}^3(c_1^*)| - 1) = 9m. \end{aligned}$$

and

$$\begin{aligned} W_p(H^f(n, m)) &= 9m + W_p(H^f(n-1, m)) \\ &= 9m + 9m + W_p(H^f(n-2, m)) \\ &= \dots \\ &= 9m \times (n-1) + W_p(H^f(1, m)) \\ &= 9nm - 2 \end{aligned}$$

for $m \geq 3$. It is easy to check $W_p(H^f(n, 1)) = 9n - 2$ and $W_p(H^f(n, 2)) = 18n - 2$, and hence $W_p(H^f(n, m)) = 9nm - 2$ for $n \geq 2$ and $m \geq 1$. Furthermore, we have $W_p(H^f(1, m)) = 9m - 2$. Thus we conclude that $W_p(H^f(n, m)) = 9nm - 2$ for $n \geq 1$ and $m \geq 1$.

Remark 3 For small values of n and m , direct computation yields

$$W_p(H^t(1, 1)) = 4, W_p(H^t(1, 2)) = W_p(H^t(2, 1)) = 18, W_p(H^t(2, 2)) = 54.$$

The Wiener polarity index of the triangular lattices

We now turn our attention to the Wiener polarity index of the triangular lattices. Again our notations follow [50]. The triangular lattices with toroidal, cylindrical and free boundary conditions are respectively denoted by $T^t(n, m)$, $T^c(n, m)$ and $T^f(n, m)$. It is not hard to see, that the triangular lattice with toroidal boundary condition $T^t(n, m)$ can be considered as an $n \times m$ square lattice $C_n \square C_m$ with toroidal boundary condition with an additional diagonal edge added to every square. As in Fig 3, $(a_1, a_1^*), (a_2, a_2^*), \dots, (a_m, a_m^*); (b_1, b_1^*), (b_2, b_2^*), \dots, (b_n, b_n^*); (b_2, b_1^*), (b_3, b_2^*), \dots, (b_n, b_{n-1}^*), (b_1, b_n^*) = (a_1, a_m^*); (a_2, a_1^*), (a_3, a_2^*), \dots, (a_m, a_{m-1}^*)$ are edges. Note that $a_1 = b_1, a_1^* = b_n, a_m = b_1^*$ and $a_m^* = b_n^*$. The triangular lattice with cylindrical boundary condition $T^c(n, m)$ is obtained by deleting the edges $(b_1, b_1^*), (b_2, b_2^*), \dots, (b_n, b_n^*); (b_2, b_1^*), (b_3, b_2^*), \dots, (b_n, b_{n-1}^*), (b_1, b_n^*)$ from $T^t(n, m)$. If we further remove the edges $(a_1, a_1^*), (a_2, a_2^*), \dots, (a_m, a_m^*); (a_2, a_1^*), (a_3, a_2^*), \dots, (a_m, a_{m-1}^*)$ from $T^c(n, m)$, the triangular lattice with free boundary condition $T^f(n, m)$ is then obtained. Since it has been established that $C_n \square C_m$ exists for $n \geq 3$ and $m \geq 3$, in what follows we assume $n \geq 3$ and $m \geq 3$ for all the triangular lattices considered.

Theorem 3 Let $T^f(n, m)$, $T^c(n, m)$ and $T^t(n, m)$ be the triangular lattices with free, cylindrical and toroidal boundary conditions respectively. Then we have

(i) For $n \geq 3$ and $m \geq 3$, $W_p(T^f(n, m)) = 9nm - 18n - 18m + 31$;

(ii)

$$W_p(T^c(n, m)) = \begin{cases} 9m - 27 & \text{if } n = 3, m \geq 3; \\ 20m - 56 & \text{if } n = 4, m \geq 3; \\ 35m - 85 & \text{if } n = 5, m \geq 3; \\ 51m - 108 & \text{if } n = 6, m \geq 3; \\ 9nm - 18n & \text{if } n \geq 7, m \geq 3; \end{cases}$$

(iii)

$$W_p(T^t(n, m)) = \begin{cases} 9m & \text{if } n = 3, m \geq 7; \\ 20m & \text{if } n = 4, m \geq 7; \\ 35m & \text{if } n = 5, m \geq 7; \\ 51m & \text{if } n = 6, m \geq 7; \\ 9nm & \text{if } n \geq 7, m \geq 7. \end{cases}$$

Moreover, for small values of n and m we have the followings:

$$W_p(T^t(n, m)) = 0 \text{ if } n = 3, 3 \leq m \leq 5 \text{ or } n = m = 4;$$

$$W_p(T^t(3, 6)) = 27; W_p(T^t(4, 5)) = 20; W_p(T^t(4, 6)) = 72;$$

$$W_p(T^t(5, 5)) = 75; W_p(T^t(5, 6)) = 165; W_p(T^t(6, 6)) = 270.$$

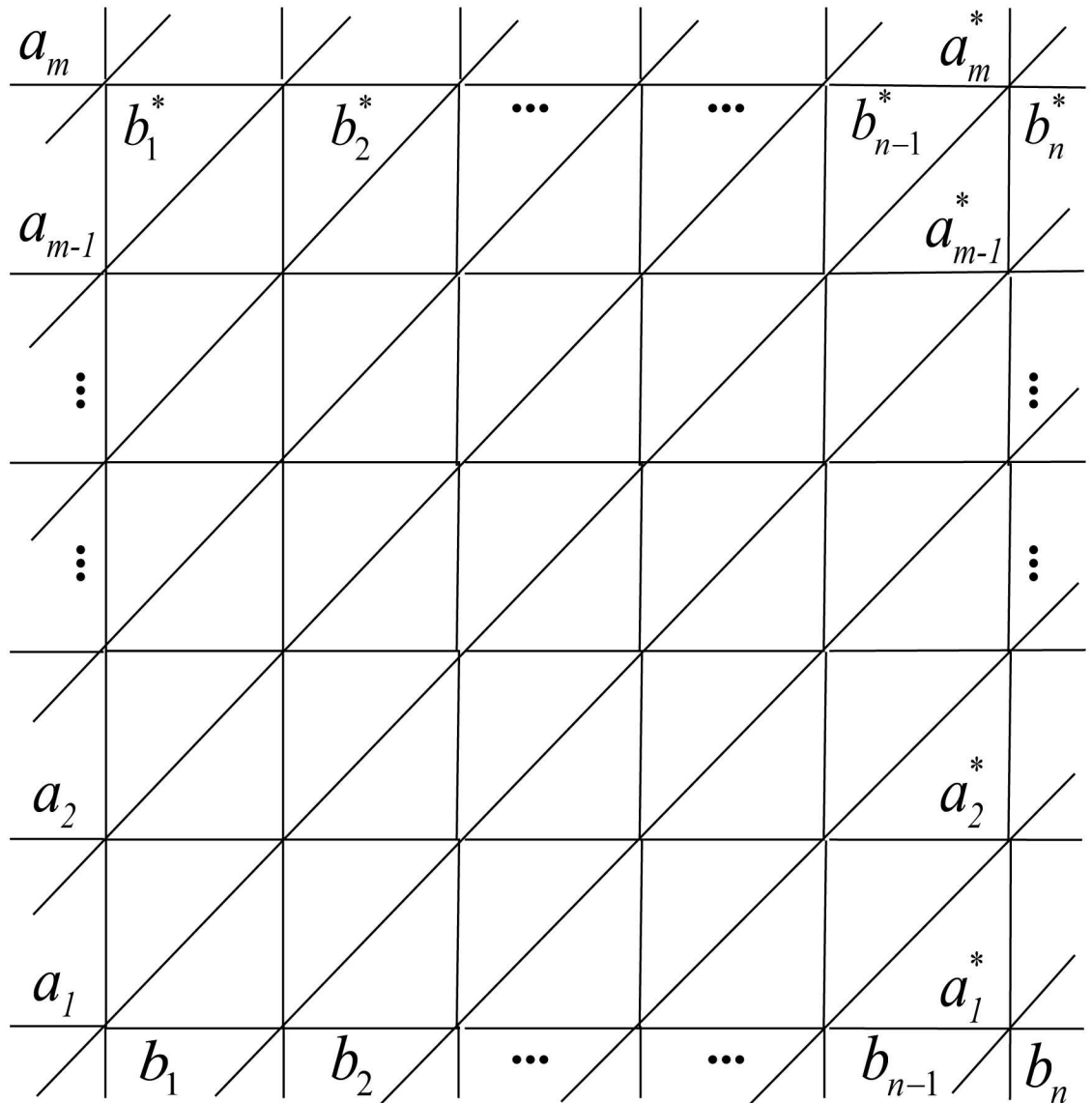


Fig 3. The triangular lattice.

doi:10.1371/journal.pone.0167075.g003

Remark 4 As illustrated in Fig 4, we generally have

$$W_p(T^t(n, m)) > W_p(T^c(n, m)) > W_p(T^f(n, m)),$$

with the common asymptotic value $9mn$ as both m and n approaches infinity. It is interesting to note that the Wiener polarity index of the triangular lattices and that of the hexagonal lattices are approximately the same.

Proof. We consider each of the three statements.

(i) First we consider the triangular lattice with free boundary condition, $T^f(n, m)$, with the assumption $n \geq m$.

Case 1 When $m = 3$:

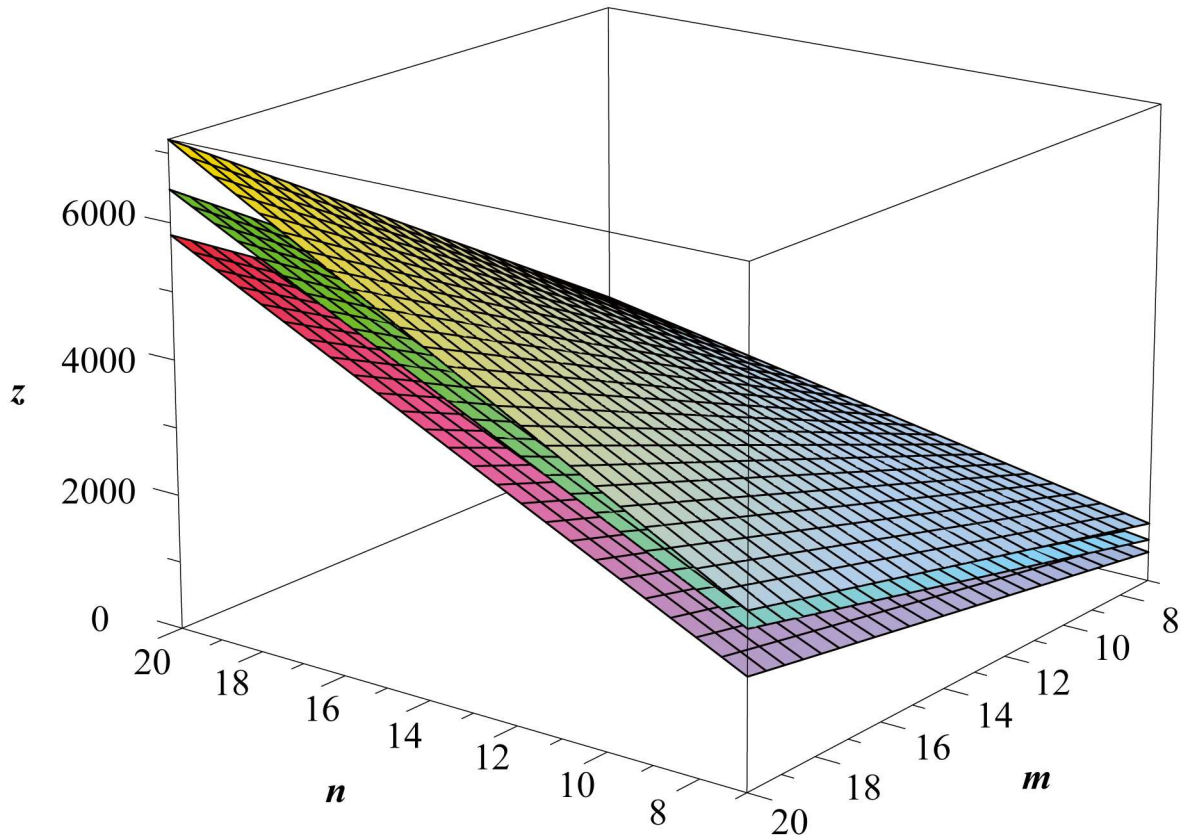


Fig 4. The Wiener polarity index of $T^f(n, m)$, $T^c(n, m)$ and $T^f(n, m)$.

doi:10.1371/journal.pone.0167075.g004

- If $n = 3$, $W_p(T^f(3, 3)) = 4$.
- If $n \geq 4$, we have

$$|N_{T^f(n,3)}^3(a_1)| = 3; \quad |N_{T^f(n,3)}^3(a_2)| = 3; \quad |N_{T^f(n,3)}^3(a_3)| = 3.$$

Thus

$$\begin{aligned} W_p(T^f(n, 3)) &= \sum_{i=1}^3 |N_{T^f(n,3)}^3(a_i)| + W_p(T^f(n-1, 3)) \\ &= 9 + W_p(T^f(n-1, 3)) \\ &= 9 + \sum_{i=1}^3 |N_{T^f(n-1,3)}^3(a_i)| + W_p(T^f(n-2, 3)) \\ &= 9 + 9 + W_p(T^f(n-2, 3)) \\ &= \dots \\ &= 9(n-3) + W_p(T^f(3, 3)) = 9n - 23, \end{aligned}$$

also satisfied by $W_p(T^f(3, 3)) = 4$.

Case 2 When $m = 4$, for $n \geq m$ we have

$$|N_{T^f(n,4)}^3(a_1)| = 7; |N_{T^f(n,4)}^3(a_2)| = 4; |N_{T^f(n,4)}^3(a_3)| = 4; |N_{T^f(n,4)}^3(a_4)| = 4.$$

Hence

$$\begin{aligned} W_p(T^f(n, 4)) &= \sum_{i=1}^4 |N_{T^f(n,4)}^3(a_i)| - W_p(P_4) + W_p(T^f(n - 1, 4)) \\ &= (19 - 1) + W_p(T^f(n - 1, 4)) \\ &= 18 + \sum_{i=1}^4 |N_{T^f(n-1,4)}^3(a_i)| - W_p(P_4) + W_p(T^f(n - 2, 4)) \\ &= 18 + 18 + W_p(T^f(n - 2, 4)) \\ &= \dots \\ &= 18(n - 3) + W_p(T^f(3, 4)) \\ &= 18(n - 3) + W_p(T^f(4, 3)) \\ &= 18n - 41. \end{aligned}$$

Case 3 When $m = 5$, similar to Case 2 we have $W_p(T^f(n, 5)) = 27n - 59$ for $n \geq m = 5$.

Case 4 When $m \geq 6$ and $n \geq m$. Simple computation yields

$$|N_{T^f(n,m)}^3(a_1)| = 7; |N_{T^f(n,m)}^3(a_2)| = 8; |N_{T^f(n,m)}^3(a_3)| = 9;$$

$$|N_{T^f(n,m)}^3(a_4)| = \dots = |N_{T^f(n,m)}^3(a_{m-3})| = 10;$$

$$|N_{T^f(n,m)}^3(a_{m-2})| = 6; |N_{T^f(n,m)}^3(a_{m-1})| = 5; |N_{T^f(n,m)}^3(a_m)| = 4.$$

Noting that $W_p(P_m) = m - 3$ and $W_p(T^f(3, m)) = W_p(T^f(m, 3)) = 9m - 23$, we have

$$\begin{aligned} W_p(T^f(n, m)) &= \sum_{i=1}^m |N_{T^f(n,m)}^3(a_i)| - W_p(P_m) + W_p(T^f(n - 1, m)) \\ &= (10m - 21) - (m - 3) + W_p(T^f(n - 1, m)) \\ &= (9m - 18) + \sum_{i=1}^m |N_{T^f(n-1,m)}^3(a_i)| - W_p(P_m) \\ &\quad + W_p(T^f(n - 2, m)) \\ &= (9m - 18) + (9m - 18) + W_p(T^f(n - 2, m)) \\ &= \dots \\ &= (9m - 18) \times (n - 3) + W_p(T^f(3, m)) \\ &= 9nm - 18n - 18m + 31. \end{aligned}$$

Since this formula coincides with our findings for smaller values of m , we conclude that $W_p(T^f(n, m)) = 9nm - 18n - 18m + 31$ for $n \geq 3$ and $m \geq 3$.

(ii) Next we consider the triangular lattice with cylindrical boundary condition $T^c(n, m)$. The symmetric structure of $T^c(n, m)$ indicates that the vertices from the same row have the same number of 3rd neighbors. Thus it suffices to compute $N_{T^c(n,m)}^3(a_i)$ for $i = 1, 2, \dots, m$ to obtain $W_p(T^c(n, m))$.

Case 1 If $n = 3$; first suppose $m \geq 7$. Direct computation yields

$$|N_{T^c(3,m)}^3(a_i)| = 3 \text{ for } i = 1, 2, 3, m - 2, m - 1, m$$

and

$$|N_{T^c(3,m)}^3(a_i)| = 6 \text{ for } 4 \leq i \leq m - 3.$$

Thus Lemma 4 implies that

$$\begin{aligned} W_p(T^c(3, m)) &= \frac{\sum_{v \in V(T^c(3,m))} |N_{T^c(3,m)}^3(v)|}{2} \\ &= \frac{\left(\sum_{i=1}^m |N_{T^c(3,m)}^3(a_i)|\right) \times 3}{2} \\ &= 9m - 27. \end{aligned}$$

On the other hand, for $3 \leq m \leq 6$, one can verify $W_p(T^c(3, m)) = 9m - 27$ through direct computation.

Case 2 If $n = 4, 5, \text{ or } 6$; Following essentially the same arguments as that of Case 1, we have

$$W_p(T^c(4, m)) = 20m - 56 \text{ for } m \geq 3;$$

$$W_p(T^c(5, m)) = 35m - 85 \text{ for } m \geq 3;$$

$$W_p(T^c(6, m)) = 51m - 108 \text{ for } m \geq 3.$$

Case 3 If $n \geq 7$:

- When $m = 3$, it is easy to see that $|N_{T^c(n,3)}^3(a_i)| = 6$ for $i = 1, 2, 3$, and hence Lemma 4 implies

$$\begin{aligned} W_p(T^c(n, 3)) &= \frac{\sum_{v \in V(T^c(n,3))} |N_{T^c(n,3)}^3(v)|}{2} \\ &= \frac{\left(\sum_{i=1}^3 |N_{T^c(n,3)}^3(a_i)|\right) \times n}{2} \\ &= 9n. \end{aligned}$$

- When $m = 4$, we have $|N_{T^c(n,4)}^3(a_1)| = |N_{T^c(n,4)}^3(a_4)| = 10$ and $|N_{T^c(n,4)}^3(a_2)| = |N_{T^c(n,4)}^3(a_3)| = 8$. Thus

$$\begin{aligned} W_p(T^c(n, 4)) &= \frac{\sum_{v \in V(T^c(n,4))} |N_{T^c(n,4)}^3(v)|}{2} \\ &= \frac{\left(\sum_{i=1}^4 |N_{T^c(n,4)}^3(a_i)|\right) \times n}{2} \\ &= 18n. \end{aligned}$$

- Similarly, when $m = 5$ or 6 we have

$$W_p(T^c(n, 5)) = 27n;$$

$$W_p(T^c(n, 6)) = 36n.$$

- When $m \geq 7$, examining the 3rd neighborhoods yields

$$|N_{T^c(n,m)}^3(a_1)| = |N_{T^c(n,m)}^3(a_m)| = 10;$$

$$|N_{T^c(n,m)}^3(a_2)| = |N_{T^c(n,m)}^3(a_{m-1})| = 12;$$

$$|N_{T^c(n,m)}^3(a_3)| = |N_{T^c(n,m)}^3(a_{m-2})| = 14;$$

$$|N_{T^c(n,m)}^3(a_i)| = 18 \text{ for } 4 \leq i \leq m - 3.$$

Consequently

$$\begin{aligned} W_p(T^c(n, m)) &= \frac{\sum_{v \in V(T^c(n,m))} |N_{T^c(n,m)}^3(v)|}{2} \\ &= \frac{\left(\sum_{i=1}^m |N_{T^c(n,m)}^3(a_i)|\right) \times n}{2} \\ &= 9nm - 18n. \end{aligned}$$

Again this formula can be verified with $m = 3, 4, 5, 6$, and hence we may conclude that $W_p(T^c(n, m)) = 9nm - 18n$ for $n \geq 7$ and $m \geq 3$.

(iii) Lastly, we consider $T^t(n, m)$ with the assumption that $m \geq n$. It is easy to see that all vertices share the same number of 3rd neighbors.

For small values of n and m , we have $W_p(T^t(n, m)) = 0$ for $n = 3$ and $3 \leq m \leq 5$ or $n = m = 4$; $W_p(T^t(3, 6)) = 27$; $W_p(T^t(4, 5)) = 20$; $W_p(T^t(4, 6)) = 72$; $W_p(T^t(5, 5)) = 75$; $W_p(T^t(5, 6)) = 165$; $W_p(T^t(6, 6)) = 270$.

For $m \geq 7$ we consider different cases depending on the value of n .

- If $n = 3$ and $m \geq 7$, then $|N_{T^t(3,m)}^3(v)| = 6$ for any vertex $v \in V(T^t(3, m))$ and

$$\begin{aligned} W_p(T^t(3, m)) &= \frac{\sum_{v \in V(T^t(3,m))} |N_{T^t(3,m)}^3(v)|}{2} \\ &= \frac{6 \times 3m}{2} \\ &= 9m. \end{aligned}$$

- If $n = 4$ and $m \geq 7$, $|N_{T^t(4,m)}^3(v)| = 10$ for any vertex $v \in V(T^t(4, m))$ and $W_p(T^t(4, m)) = 20m$.

- If $n = 5$ and $m \geq 7$, $|N_{T^t(5,m)}^3(v)| = 14$ for any vertex $v \in V(T^t(5, m))$ and $W_p(T^t(5, m)) = 35m$.

- If $n = 6$ and $m \geq 7$, $|N_{T^t(6,m)}^3(v)| = 17$ for any vertex $v \in V(T^t(6, m))$ and $W_p(T^t(6, m)) = 51m$.

- If $n \geq 7$ and $m \geq 7$, direct computation shows $|N_{T^t(n,m)}^3(v)| = 18$ for any vertex $v \in V(T^t(n, m))$. Hence

$$\begin{aligned} W_p(T^t(n, m)) &= \frac{\sum_{v \in V(T^t(n,m))} |N_{T^t(n,m)}^3(v)|}{2} \\ &= \frac{18 \times nm}{2} \\ &= 9nm. \end{aligned}$$

The Wiener polarity index of the $3^3 \cdot 4^2$ lattices

We conclude our study by considering the Wiener polarity index of the $3^3 \cdot 4^2$ lattices, following the notations of [50]. The $3^3 \cdot 4^2$ lattice with toroidal boundary condition, denoted by $S^t(n, 2m)$, can be constructed from the square lattice $C_{2m} \square C_n$ by adding a diagonal edge in each square of every other row, as shown in Fig 5. Here $a_1 = b_1, a_{2m} = b_1^*, a_1^* = b_n, a_{2m}^* = b_n^*$, and $(a_1, a_1^*), (a_2, a_2^*), \dots, (a_{2m}, a_{2m}^*); (b_1, b_1^*), (b_2, b_2^*), \dots, (b_n, b_n^*); (a_1, a_2^*), (a_3, a_4^*), \dots, (a_{2m-1}, a_{2m}^*)$ are edges. If we remove the edges $(b_1, b_1^*), (b_2, b_2^*), \dots, (b_n, b_n^*)$ of $S^t(n, 2m)$, then the $3^3 \cdot 4^2$ lattice with cylindrical boundary condition, denoted by $S^c(n, 2m)$, is obtained. The $3^3 \cdot 4^2$ lattice $S^f(n, 2m)$ with free boundary condition is obtained by further removing edges $(a_1, a_1^*), (a_2, a_2^*), \dots, (a_{2m}, a_{2m}^*); (a_1, a_2^*), (a_3, a_4^*), \dots, (a_{2m-1}, a_{2m}^*)$ from $S^c(n, 2m)$. Similar to before, we will assume $n \geq 3$ and $m \geq 2$ when the $3^3 \cdot 4^2$ lattices are discussed.

Theorem 4 Let $S^f(n, 2m), S^c(n, 2m)$ and $S^t(n, 2m)$ be the $3^3 \cdot 4^2$ lattices with free, cylindrical and toroidal boundary conditions, respectively. Then

- (i) For $n \geq 3$ and $m \geq 2$, $W_p(S^f(n, 2m)) = 15nm - 13n - 25m + 15$;
- (ii)

$$W_p(S^c(n, 2m)) = \begin{cases} 21m - 27 & \text{if } n = 3, m \geq 2; \\ 40m - 48 & \text{if } n = 4, m \geq 2; \\ 60m - 65 & \text{if } n = 5, m \geq 2; \\ 84m - 78 & \text{if } n = 6, m \geq 2; \\ 15nm - 13n & \text{if } n \geq 7, m \geq 2; \end{cases}$$

- (iii)

$$W_p(S^t(n, 2m)) = \begin{cases} 21m & \text{if } n = 3, m \geq 4; \\ 40m & \text{if } n = 4, m \geq 4; \\ 60m & \text{if } n = 5, m \geq 4; \\ 84m & \text{if } n = 6, m \geq 4; \\ 16n & \text{if } n \geq 7, m = 2; \\ 42n & \text{if } n \geq 7, m = 3; \\ 15nm & \text{if } n \geq 7, m \geq 4. \end{cases}$$

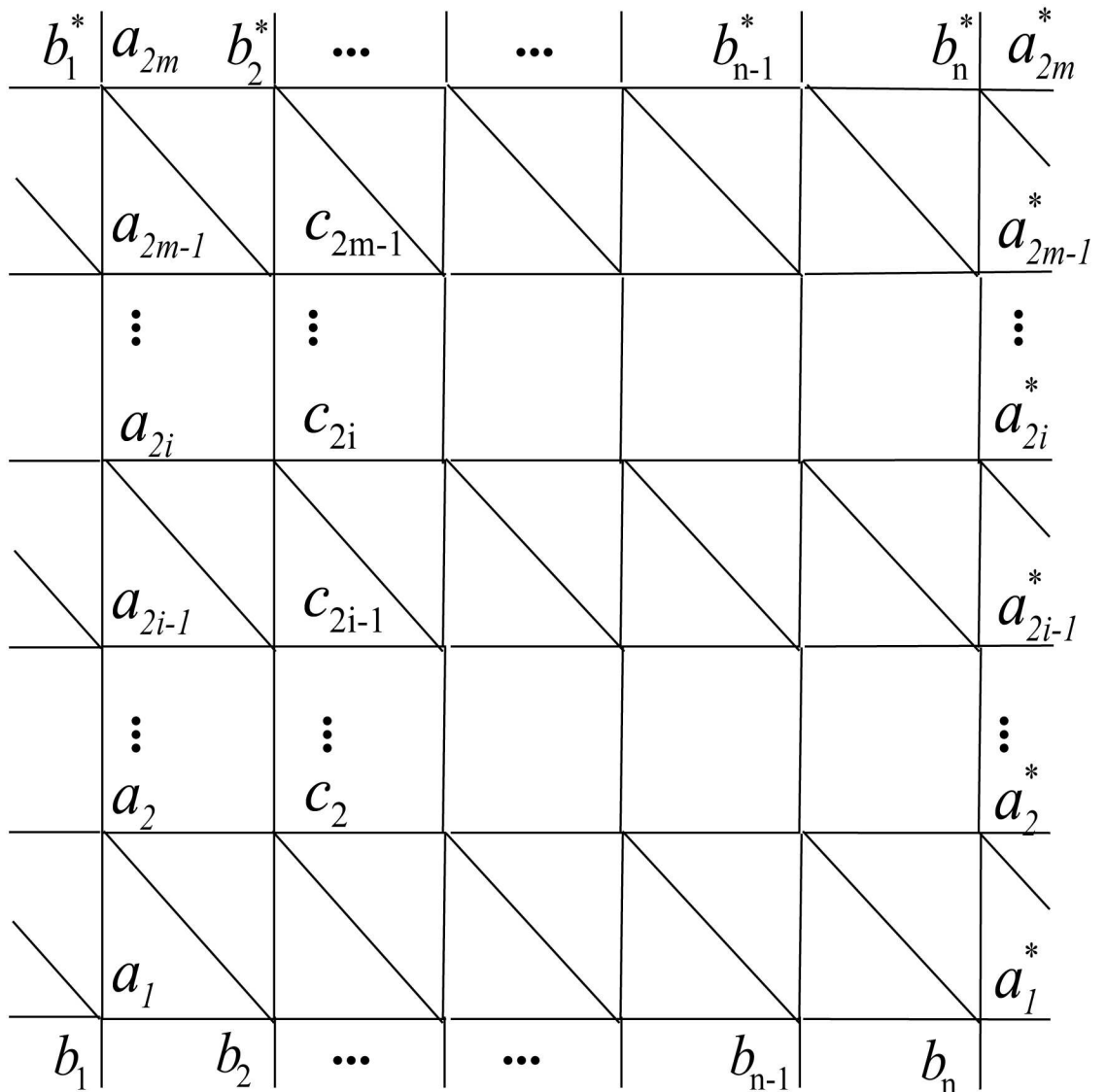


Fig 5. The $3^3 \cdot 4^2$ lattice.

doi:10.1371/journal.pone.0167075.g005

In addition, for small n and m we have $W_p(S^t(3, 4)) = 0$; $W_p(S^t(3, 6)) = 45$; $W_p(S^t(4, 4)) = 16$; $W_p(S^t(4, 6)) = 108$; $W_p(S^t(5, 4)) = 50$; $W_p(S^t(5, 6)) = 165$; $W_p(S^t(6, 4)) = 84$; $W_p(S^t(6, 6)) = 234$.

Remark 5 As illustrated in Fig 6, we generally have

$$W_p(S^t(n, m)) > W_p(S^c(n, m)) > W_p(S^f(n, m)),$$

with the common asymptotic value $15mn$ as both m and n approaches infinity.

Proof. We consider each of the three cases as follows:

(i) We start with the $3^3 \cdot 4^2$ lattice $S^f(n, 2m)$ with free boundary condition. First we consider $W_p(S^f(n, 2m))$, noting that $|N_{S^f(3,2m)}^3(a_i)| = |N_{S^f(3,2m)}^3(a_{2m+1-i}^*)|$ for $1 \leq i \leq 2m$, thus for $m \geq 4$

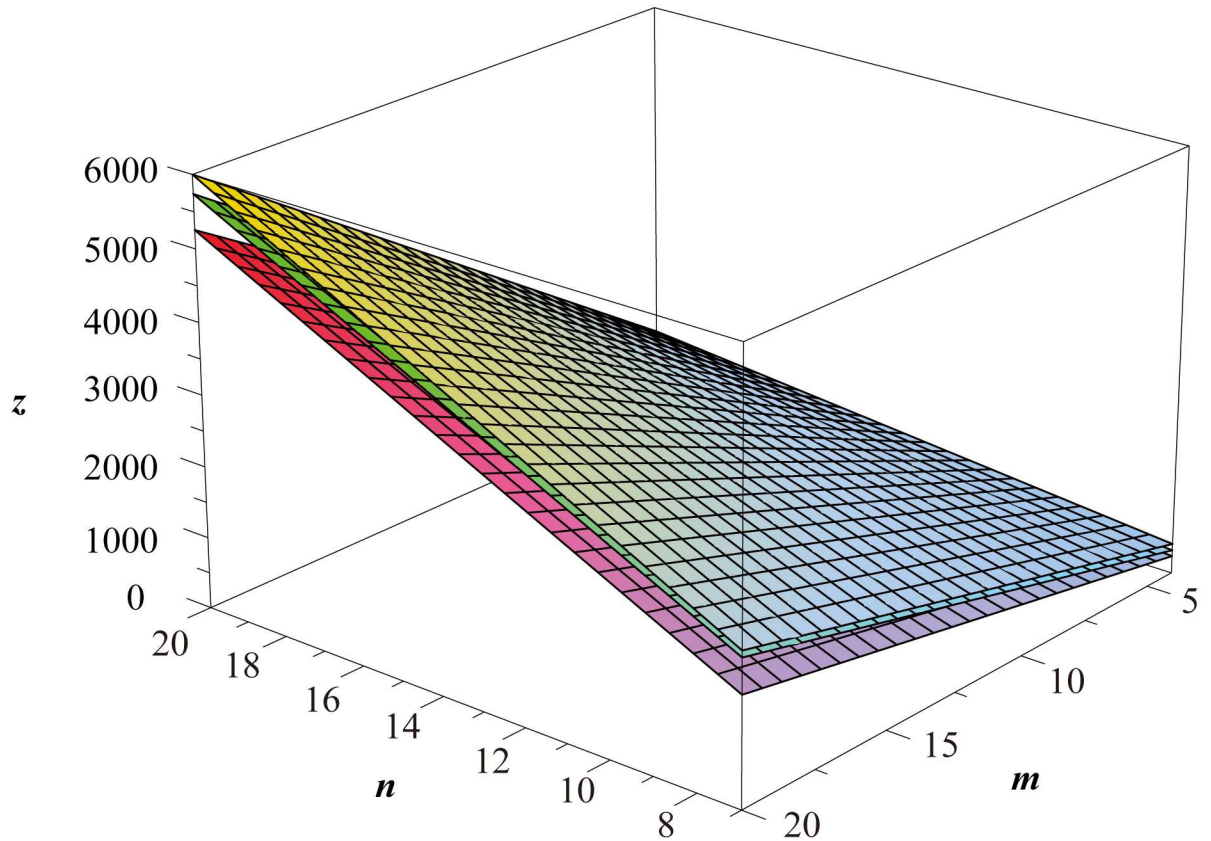


Fig 6. The Wiener polarity index of $S^f(n, m)$, $S^c(n, m)$ and $S^f(n, m)$.

doi:10.1371/journal.pone.0167075.g006

we have

$$|N_{S^f(3,2m)}^3(a_1)| = |N_{S^f(3,2m)}^3(a_{2m}^*)| = 3; \quad |N_{S^f(3,2m)}^3(a_2)| = |N_{S^f(3,2m)}^3(a_{2m-1}^*)| = 3;$$

$$|N_{S^f(3,2m)}^3(a_3)| = |N_{S^f(3,2m)}^3(a_{2m-2}^*)| = 5; \quad |N_{S^f(3,2m)}^3(a_{2m-2})| = |N_{S^f(3,2m)}^3(a_3^*)| = 6;$$

$$|N_{S^f(3,2m)}^3(a_{2m-1})| = |N_{S^f(3,2m)}^3(a_2^*)| = 5; \quad |N_{S^f(3,2m)}^3(a_{2m})| = |N_{S^f(3,2m)}^3(a_1^*)| = 4;$$

$$|N_{S^f(3,2m)}^3(a_i)| = |N_{S^f(3,2m)}^3(a_{2m+1-i}^*)| = 7 \quad \text{for } 4 \leq i \leq 2m - 3;$$

$$|N_{S^f(3,2m)}^3(b_2)| = 3; \quad |N_{S^f(3,2m)}^3(c_2)| = 3; \quad |N_{S^f(3,2m)}^3(c_3)| = 4;$$

$$|N_{S^f(3,2m)}^3(c_{2m-2})| = 4; \quad |N_{S^f(3,2m)}^3(c_{2m-1})| = 3; \quad |N_{S^f(3,2m)}^3(b_2^*)| = 3;$$

$$|N_{S^f(3,2m)}^3(c_i)| = 6 \quad \text{for } 4 \leq i \leq 2m - 3.$$

Plugging into Eq (2), we have $W_p(S^f(3, 2m)) = 20m - 24$ for $m \geq 4$. Since $W_p(S^f(3, 4)) = 16 = 20 \times 2 - 24$ when $m = 2$ and $W_p(S^f(3, 6)) = 36 = 20 \times 3 - 24$ when $m = 3$, we conclude that $W_p(S^f(3, 2m)) = 20m - 24$ for $m \geq 2$.

Now suppose $n \geq 4$. Observe that if the vertices in the first column are removed from $S^f(n, 2m)$, then $S^f(n-1, 2m)$ is obtained. We now consider the vertices in the first column of $S^f(n, 2m)$ and their 3rd neighbors:

$$|N_{S^f(n,2m)}^3(a_1)| = 4; |N_{S^f(n,2m)}^3(a_2)| = 5; |N_{S^f(n,2m)}^3(a_3)| = 6;$$

$$|N_{S^f(n,2m)}^3(a_i)| = 9 \quad \text{for } i = 4, 6, \dots, 2m - 4;$$

$$|N_{S^f(n,2m)}^3(a_i)| = 8 \quad \text{for } i = 5, 7, \dots, 2m - 3;$$

$$|N_{S^f(n,2m)}^3(a_{2m-2})| = 8; |N_{S^f(n,2m)}^3(a_{2m-1})| = 6; |N_{S^f(n,2m)}^3(a_{2m})| = 6;$$

Applying Lemma 4 together with the fact that $W_p(P_n) = n - 3$, have, for $m \geq 4$,

$$\begin{aligned} W_p(S^f(n, 2m)) &= \sum_{i=1}^{2m} |N_{S^f(n,2m)}^3(a_i)| - W_p(P_{2m}) + W_p(S^f(n-1, 2m)) \\ &= (15m - 13) + W_p(S^f(n-1, 2m)) \\ &= (15m - 13) + \sum_{i=1}^{2m} |N_{S^f(n-1,2m)}^3(a_i)| - W_p(P_{2m}) \\ &\quad + W_p(S^f(n-2, 2m)) \\ &= (15m - 13) + (15m - 13) + W_p(T^f(n-2, m)) \\ &= \dots \\ &= (15m - 13) \times (n - 3) + W_p(S^f(3, 2m)) \\ &= 15nm - 13n - 25m + 15. \end{aligned}$$

Again this formula can be verified for small values of n and m . Hence $W_p(S^f(n, 2m)) = 15nm - 13n - 25m + 15$ for $m \geq 2$.

(ii) Next we consider the $3^3 \cdot 4^2$ lattice $S^c(n, 2m)$ with cylindrical boundary condition. In this case the vertices of $S^c(n, 2m)$ in the same row have the same number of 3rd neighbors. Hence it is sufficient to compute $|N_{S^c(n,2m)}^3(a_i)|$ for $i = 1, 2, \dots, 2m$.

Case 1 If $n = 3$ and $m \geq 2$; When $m \geq 4$ we have

$$|N_{S^c(3,2m)}^3(a_1)| = |N_{S^c(3,2m)}^3(a_{2m})| = 4;$$

$$|N_{S^c(3,2m)}^3(a_2)| = |N_{S^c(3,2m)}^3(a_{2m-1})| = 3;$$

$$|N_{S^c(3,2m)}^3(a_3)| = |N_{S^c(3,2m)}^3(a_{2m-2})| = 5;$$

$$|N_{S^c(3,2m)}^3(a_i)| = 7 \quad \text{for } 4 \leq i \leq 2m - 3.$$

Then Lemma 4 implies

$$\begin{aligned} W_p(S^c(3, 2m)) &= \frac{\sum_{v \in V(S^c(3, 2m))} |N_{S^c(3, 2m)}^3(v)|}{2} \\ &= \frac{\left(\sum_{i=1}^{2m} |N_{S^c(3, 2m)}^3(a_i)|\right) \times 3}{2} \\ &= 21m - 27. \end{aligned}$$

This formula can be easily verified for $W_p(S^c(3, 4)) = 15$ ($m = 2$) and $W_p(S^c(3, 6)) = 36$ ($m = 3$).

Case 2 If $n = 4$ and $m \geq 2$; When $m \geq 4$, we have

$$|N_{S^c(4, 2m)}^3(a_i)| = 5 \quad \text{for } i = 1, 2, 2m - 1, 2m;$$

$$|N_{S^c(4, 2m)}^3(a_3)| = |N_{S^c(4, 2m)}^3(a_{2m-2})| = 8;$$

$$|N_{S^c(4, 2m)}^3(a_i)| = 10 \quad \text{for } 4 \leq i \leq 2m - 3.$$

Thus

$$\begin{aligned} W_p(S^c(4, 2m)) &= \frac{\sum_{v \in V(S^c(4, 2m))} |N_{S^c(4, 2m)}^3(v)|}{2} \\ &= \frac{\left(\sum_{i=1}^{2m} |N_{S^c(4, 2m)}^3(a_i)|\right) \times 4}{2} \\ &= 40m - 48. \end{aligned}$$

Again this can be verified for $m = 2$ or 3 .

Case 3 Similarly, we have

$$W_p(S^c(n, 2m)) = 60m - 65 \quad \text{for } n = 5 \quad \text{and } m \geq 2;$$

$$W_p(S^c(n, 2m)) = 84m - 78 \quad \text{for } n = 6 \quad \text{and } m \geq 2.$$

Case 4 If $n \geq 7$ and $m \geq 2$;

- When $m = 2$ and $n \geq 7$, we have

$$|N_{S^c(n, 4)}^3(a_1)| = |N_{S^c(n, 4)}^3(a_4)| = 9; \quad |N_{S^c(n, 4)}^3(a_2)| = |N_{S^c(n, 4)}^3(a_3)| = 8.$$

Hence

$$\begin{aligned} W_p(S^c(n, 4)) &= \frac{\sum_{v \in V(S^c(n, 4))} |N_{S^c(n, 4)}^3(v)|}{2} \\ &= \frac{\left(\sum_{i=1}^4 |N_{S^c(n, 4)}^3(a_i)|\right) \times n}{2} \\ &= 17n. \end{aligned}$$

- When $m = 3$, we have

$$|N_{S^c(n, 6)}^3(a_1)| = |N_{S^c(n, 6)}^3(a_6)| = 9;$$

$$|N_{S^c(n, 6)}^3(a_2)| = |N_{S^c(n, 6)}^3(a_5)| = 10;$$

$$|N_{S^c(n, 6)}^3(a_3)| = |N_{S^c(n, 6)}^3(a_4)| = 13.$$

and hence $W_p(S^c(n, 6)) = 32n$.

- When $m \geq 4$, we have

$$|N_{S^c(n, 2m)}^3(a_1)| = |N_{S^c(n, 2m)}^3(a_{2m})| = 9;$$

$$|N_{S^c(n, 2m)}^3(a_2)| = |N_{S^c(n, 2m)}^3(a_{2m-1})| = 10;$$

$$|N_{S^c(n, 2m)}^3(a_3)| = |N_{S^c(n, 2m)}^3(a_{2m-2})| = 13;$$

$$|N_{S^c(n, 2m)}^3(a_i)| = 15 \text{ for } 4 \leq i \leq 2m - 3.$$

Hence

$$\begin{aligned} W_p(S^c(n, 2m)) &= \frac{\sum_{v \in V(S^c(n, 2m))} |N_{S^c(n, 2m)}^3(v)|}{2} \\ &= \frac{\left(\sum_{i=1}^{2m} |N_{S^c(n, 2m)}^3(a_i)|\right) \times n}{2} \\ &= 15nm - 13n. \end{aligned}$$

Note that the formula $W_p(S^c(n, 2m)) = 15nm - 13n$ also hold for both $m = 2$ and $m = 3$.

(iii) Lastly, we calculate the Wiener polarity index of $S^t(n, 2m)$, the $3^3 \cdot 4^2$ lattice with toroidal boundary condition. As in $H^t(n, m)$ and $T^t(n, m)$, all vertices of $S^t(n, 2m)$ have the same number of 3rd neighbors. Also note that $|V(S^t(n, 2m))| = 2nm$.

Case 1 If $n = 3$ and $m \geq 2$, it is easy to see that $W_p(S^t(3, 4)) = 0$ and $W_p(S^t(3, 6)) = 45$. When $m \geq 4$, we have $|N_{S^t(3,2m)}^3(v)| = 7$ for any $v \in V(S^t(3, 2m))$. Hence

$$\begin{aligned} W_p(S^t(3, 2m)) &= \frac{\sum_{v \in V(S^t(3,2m))} |N_v^3(v)|}{2} \\ &= \frac{7 \times |V(S^t(3, 2m))|}{2} \\ &= 21m. \end{aligned}$$

Case 2 If $n = 4$ and $m \geq 2$;

- When $m = 2$, we have $W_p(S^t(4, 4)) = 16$.
- When $m = 3$, we have $W_p(S^t(4, 6)) = 108$.
- When $m \geq 4$, we have $|V(S^t(4, 2m))| = 8m$ and $|N_{S^t(4,2m)}^3(v)| = 10$ for any $v \in V(S^t(4, 2m))$. Hence $W_p(S^t(4, 2m)) = 40m$ by Lemma 4.

Case 3 If $n = 5$ and $m \geq 2$, similarly we have

$$W_p(S^t(5, 4)) = 50; \quad W_p(S^t(5, 6)) = 165;$$

and

$$W_p(S^t(5, 2m)) = 60m \quad \text{for } m \geq 4;$$

Case 4 If $n = 6$ and $m \geq 2$, similarly we have

$$W_p(S^t(6, 4)) = 84; \quad W_p(S^t(6, 6)) = 234;$$

and

$$W_p(S^t(6, 2m)) = 84m \quad \text{for } m \geq 4.$$

Case 5 If $n \geq 7$ and $m \geq 2$:

- When $m = 2$, we have $|N_{S^t(n,4)}^3(v)| = 8$ for any $v \in V(S^t(n, 4))$ and $W_p(S^t(n, 4)) = 16n$.
- When $m = 3$, we have $|N_{S^t(n,6)}^3(v)| = 14$ for any $v \in V(S^t(n, 6))$ and $W_p(S^t(n, 6)) = 42n$.
- When $m \geq 4$, we have $|N_{S^t(n,2m)}^3(v)| = 15$ for any $v \in V(S^t(n, 2m))$ and hence

$$\begin{aligned} W_p(S^t(n, 2m)) &= \frac{\sum_{v \in V(S^t(n,2m))} |N_{S^t(n,2m)}^3(v)|}{2} \\ &= \frac{15 \times |V(S^t(n, 2m))|}{2} \\ &= 15nm. \end{aligned}$$

Concluding remarks

Evaluation of topological indices of network structures is an important problem in the study of network robustness [71–73]. In particular, the computation of distance-based graph indices of various lattices has attracted the attention of researchers from many different backgrounds. By using a fundamental general formula of the Wiener polarity index of graphs, we determined

the explicit formulas for the Wiener polarity index of the square lattices, the hexagonal lattices, the triangular lattices, and the $3^3 \cdot 4^2$ lattices with free, cylindrical and toroidal boundary conditions. The results of Theorems 2, 3, and 4 are plotted in Figs 4–6 respectively.

There exist other interesting graph structures of practical interests, such as the polyomino chains and the triangular Kagomé lattices. It would be worthwhile to explore their structure through computation of similar graph indices [74–77]. Given our findings, it may also be interesting to study the asymptotic behavior of a given topological index of these lattices structures. Furthermore, it could be a challenge to develop theoretical bounds on such indices, when certain restrictions (such as the sizes and number of “holes” in a hexagonal system) accommodated by the graph structure.

Author Contributions

Conceptualization: LC TL JL YS HW.

Data curation: LC TL JL YS HW.

Formal analysis: LC TL JL YS HW.

Funding acquisition: LC TL JL YS HW.

Investigation: LC TL JL YS HW.

Methodology: LC TL JL YS HW.

Project administration: LC TL JL YS HW.

Resources: LC TL JL YS HW.

Software: TL.

Supervision: LC TL JL YS HW.

Validation: LC TL JL YS HW.

Visualization: LC TL JL YS HW.

Writing – original draft: LC TL JL YS HW.

Writing – review & editing: LC TL JL YS HW.

References

1. Boccaletti S, Latora V, Moreno Y, Chavez M, Hwang D (2006) Complex networks: structure and dynamics. *Physics Reports* 424: 175–308. doi: [10.1016/j.physrep.2005.10.009](https://doi.org/10.1016/j.physrep.2005.10.009)
2. Costa L. da F., Rodrigues F, Trivieso G, Villas Boas PR, Characterization of complex networks: A survey of measurements, *Adv. Phys.* 56 (2007) 167–242. doi: [10.1080/00018730601170527](https://doi.org/10.1080/00018730601170527)
3. Dorogovtsev S, Mendes J (2002) Evolution of networks. *Adv Phys* 51: 1079–1187. doi: [10.1080/00018730110112519](https://doi.org/10.1080/00018730110112519)
4. Ellens W, Kooij R (2013) Graph measures and network robustness. arXiv:1311.5064v1 [cs. DM].
5. Gutman I, Li X, Zhang J, (2009) Graph energy, in: Dehmer M, Emmert-Streib F(Eds.). *Analysis of Complex Networks—From Biology to Linguistics*. Wiley-VCH, Weinheim, pp. 145–174.
6. Kraus V, Dehmer M, Emmert-Streib F (2014) Probabilistic inequalities for evaluating structural network measures. *Inform Sciences* 288: 220–245. doi: [10.1016/j.ins.2014.07.018](https://doi.org/10.1016/j.ins.2014.07.018)
7. Sydney A, Scoglio C, Schumm P, Kooij R (2008) Elasticity: topological characterization of robustness in complex networks. *IEEE/ACM Bionetics*. doi: [10.4108/ICST.BIONETICS2008.4713](https://doi.org/10.4108/ICST.BIONETICS2008.4713)
8. Hosoya H (1971) Topological index, a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. *Bull Chem Soc Jpn* 44: 2332–2339. doi: [10.1246/bcsj.44.2332](https://doi.org/10.1246/bcsj.44.2332)

9. Bollobás B, Erdős P (1998) Graphs of extremal weights. *Ars Combin* 50: 225–233.
10. Li X, Shi Y (2008) A survey on the Randić index. *MATCH Commun Math Comput Chem* 59: 127–156.
11. Randić M (1975) On characterization of molecular branching. *J Amer Chem Soc* 97: 6609–6615. doi: [10.1021/ja00856a001](https://doi.org/10.1021/ja00856a001)
12. Kier LB, Hall LH (1977) The nature of structure-activity relationships and their relation to molecular connectivity. *Europ J Med Chem* 12: 307–312.
13. Li X, Zheng J (2005) A unified approach to the extremal trees for different indices. *MATCH Commun Math Comput Chem* 54: 195–208.
14. Gutman I, Ruščić B, Trinajstić N, Wilcox CF (1975) Graph theory and molecular orbitals. XII. Acyclic polyenes. *J Chem Phys* 62: 3399–3405. doi: [10.1063/1.430994](https://doi.org/10.1063/1.430994)
15. Gutman I, Trinajstić N (1972) Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons. *Chem Phys Lett* 17: 535–538. doi: [10.1016/0009-2614\(72\)85099-1](https://doi.org/10.1016/0009-2614(72)85099-1)
16. Gupta S, Singh M, Madan AK (2000) Connective eccentricity index: a novel topological descriptor for predicting biological activity. *J Mol Graph Model* 18: 18–25. doi: [10.1016/S1093-3263\(00\)00027-9](https://doi.org/10.1016/S1093-3263(00)00027-9) PMID: [10935202](https://pubmed.ncbi.nlm.nih.gov/10935202/)
17. Rada J, Cruz R, Gutman I (2014) Benzenoid systems with extremal vertex-degree-based topological indices. *MATCH Commun Math Comput Chem* 72: 125–136.
18. Xu K, Liu M, Das KC, Gutman I, Furtula B (2014) A survey on graphs extremal with respect to distance-based topological indices. *MATCH Commun Math Comput Chem* 71(3): 461–508.
19. Balaban AT (1982) Highly discriminating distance based numerical descriptor. *Chem Phys Lett* 89: 399–404. doi: [10.1016/0009-2614\(82\)80009-2](https://doi.org/10.1016/0009-2614(82)80009-2)
20. Balaban AT (1983) Topological indices based on topological distances in molecular graphs. *Pure Appl Chem* 55: 199–206. doi: [10.1351/pac198855020199](https://doi.org/10.1351/pac198855020199)
21. Wiener H (1947) Structural determination of paraffin boiling points. *J Am Chem Soc* 69: 17–20. doi: [10.1021/ja01193a005](https://doi.org/10.1021/ja01193a005) PMID: [20291038](https://pubmed.ncbi.nlm.nih.gov/20291038/)
22. Klein DJ, Randić M (1993) Resistance distance. *J Math Chem* 12: 81–95. doi: [10.1007/BF01164627](https://doi.org/10.1007/BF01164627)
23. Pirzada S, Ganie HA, Gutman I (2015) On Laplacian-energy-like invariant and Kirchhoff index. *MATCH Commun Math Comput Chem* 73: 41–59.
24. Nosal E (1970) Eigenvalues of Graphs. Master's thesis, University of Calgary.
25. Li X, Shi Y, Gutman I (2012) Graph Energy. Springer. doi: [10.1007/978-1-4614-4220-2](https://doi.org/10.1007/978-1-4614-4220-2)
26. Bozkurt SB, Güngör AD, Gutman I, Cevik AS (2010) Randić matrix and Randić energy. *MATCH Commun Math Comput Chem* 64: 239–250.
27. Gutman I (1978) The energy of a graph. *Ber Math Statist Sect Forsch Graz* 103: 1–22.
28. Gutman I, Wagner S (2012) The matching energy of a graph. *Discrete Appl Math* 160(15): 2177–2187. doi: [10.1016/j.dam.2012.06.001](https://doi.org/10.1016/j.dam.2012.06.001)
29. Jooyandeh M, Kiani D, Mirzakhah M (2009) Incidence energy of a graph. *MATCH Commun Math Comput Chem* 62: 561–572.
30. Chen L, Liu J (2016) Extremal values of matching energies of one class of graphs. *Appl Math Comput* 273: 976–992. doi: [10.1016/j.amc.2015.10.025](https://doi.org/10.1016/j.amc.2015.10.025)
31. Chen L, Liu J, Shi Y (2015) Matching energy of unicyclic and bicyclic graphs with a given diameter. *Complexity* 21: 224–238. doi: [10.1002/cplx.21599](https://doi.org/10.1002/cplx.21599)
32. Chen L, Liu J, Shi Y (2016) Bounds on the Matching Energy of Unicyclic Odd-cycle Graphs. *MATCH Commun Math Comput Chem* 75: 315–330.
33. Chen L, Shi Y (2015) The maximal matching energy of tricyclic graphs. *MATCH Commun Math Comput Chem* 73: 105–119.
34. Das KC, Sorgun S (2014) On Randić energy of graphs. *MATCH Commun Math Comput Chem* 72: 227–238.
35. Das KC, Sorgun S, Gutman I (2015) On Randić energy. *MATCH Commun Math Comput Chem* 73: 81–92.
36. Gu R, Li X, Liu J (2015) Note on three results on Randić energy and incidence energy. *MATCH Commun Math Comput Chem* 73: 61–71.
37. Jaklič G, Fowler PW, Pisanski T (2012) *HL*-index of a graph. *Ars Math Contemp* 5: 99–105.
38. Li X, Li Y, Shi Y, Gutman I (2013) Note on the HOMO-LUMO index of graphs. *MATCH Commun Math Comput Chem* 70(1): 85–96.

39. Chen X, Hou Y (2015) Some results on Laplacian Estrada index of graphs. *MATCH Commun Math Comput Chem* 73: 149–162.
40. Chen X, Qian J (2015) On resolvent Estrada index. *MATCH Commun Math Comput Chem* 73: 163–174.
41. Gao N, Qiao L, Ning B, Zhang S (2015) Coulson-type integral formulas for the Estrada index of graphs and the skew Estrada index of oriented graphs. *MATCH Commun Math Comput Chem* 73: 133–148.
42. Feng L, Liu W, Ilić A, Yu G (2013) The degree distance of unicyclic graphs with given matching number. *Graphs Combin* 29(3): 449–462. doi: [10.1007/s00373-012-1143-5](https://doi.org/10.1007/s00373-012-1143-5)
43. Cao S, Dehmer M, Shi Y (2014) Extremality of degree-based graph entropies. *Inform Sci* 278: 22–33. doi: [10.1016/j.ins.2014.03.133](https://doi.org/10.1016/j.ins.2014.03.133)
44. Chen Z, Dehmer M, Shi Y (2014) A note on distance-based graph entropies. *Entropy* 16(10): 5416–5427. doi: [10.3390/e16105416](https://doi.org/10.3390/e16105416)
45. Li S, Yan W, Tian T (2016) The spectrum and Laplacian spectrum of the dice lattice. *J Stat Phys* 164: 449–462. doi: [10.1007/s10955-016-1552-6](https://doi.org/10.1007/s10955-016-1552-6)
46. Liu J, Pan X (2015) A unified approach to the asymptotic topological indices of various lattices. *Appl Math Comput* 270: 62–73. doi: [10.1016/j.amc.2015.08.008](https://doi.org/10.1016/j.amc.2015.08.008)
47. Liu J, Pan X (2015) Asymptotic incidence energy of lattices. *Physica A* 422: 193–202. doi: [10.1016/j.physa.2014.12.006](https://doi.org/10.1016/j.physa.2014.12.006)
48. Liu J, Pan X, Hu F, Hu F (2015) Asymptotic Laplacian-energy-like invariant of lattices. *Appl Math Comput* 253: 205–214. doi: [10.1016/j.amc.2014.12.035](https://doi.org/10.1016/j.amc.2014.12.035)
49. Shrock R, Wu F (2000) Spanning trees on graphs and lattices in d dimensions. *J Phys A: Math Gen* 33: 3881–3902. doi: [10.1088/0305-4470/33/21/303](https://doi.org/10.1088/0305-4470/33/21/303)
50. Yan W, Zhang Z (2009) Asymptotic energy of lattices. *Physica A* 388: 1463–1471. doi: [10.1016/j.physa.2008.12.058](https://doi.org/10.1016/j.physa.2008.12.058)
51. Ye L (2011) On the Kirchhoff index of some toroidal lattices. *Linear Multilinear A* 59: 645–650. doi: [10.1080/03081081003794233](https://doi.org/10.1080/03081081003794233)
52. Bondy JA, Murty MSR (2008) *Graph Theory*, Springer.
53. Dobrynin AA, Gutman I, Klavžar S, Žigert P (2002) Wiener index of hexagonal systems. *Acta Appl Math* 72: 247–294. doi: [10.1023/A:1016290123303](https://doi.org/10.1023/A:1016290123303)
54. Ghebleh M, Kanso A, Stevanovic D (2016) On trees having the same Wiener index as their quadratic line graph. *MATCH Commun Math Comput Chem* 76: 731–744.
55. Khalifeh MH, Yousefi-Azari H, Ashrafi AR, Wagner SG (2009) Some new results on distance-based graph invariants. *European J Comb* 30: 1149–1163. doi: [10.1016/j.ejc.2008.09.019](https://doi.org/10.1016/j.ejc.2008.09.019)
56. Wu X, Liu H (2010) On the Wiener index of graphs. *Acta Appl Math* 110: 535–544. doi: [10.1007/s10440-009-9460-2](https://doi.org/10.1007/s10440-009-9460-2)
57. Dobrynin AA, Entringer RC, Gutman I (2001) Wiener index of trees: theory and applications. *Acta Appl Math* 66: 211–249. doi: [10.1023/A:1010767517079](https://doi.org/10.1023/A:1010767517079)
58. Lukovits I, Linert W (1998) Polarity-numbers of cycle-containing structures. *J Chem Inf Comput Sci* 38: 715–719. doi: [10.1021/ci970122j](https://doi.org/10.1021/ci970122j)
59. Hosoya H (2002) Mathematical and chemical analysis of Wiener's polarity number, in: Rouvray DH, King RB(Eds.). *Topology in Chemistry-Discrete Mathematics of Molecules*. Horwood, Chichester. doi: [10.1533/9780857099617.38](https://doi.org/10.1533/9780857099617.38)
60. Du W, Li X, Shi Y (2009) Algorithms and extremal problem on Wiener polarity index. *MATCH Commun Math Comput Chem* 62: 235–244.
61. Deng H, Xiao H, Tang F (2010) On the extremal Wiener polarity index of trees with a given diameter. *MATCH Commun Math Comput Chem* 63: 257–264.
62. Hou H, Liu B, Huang Y (2012) The maximum Wiener polarity index of unicyclic graphs. *Appl Math Comput* 218: 10149–10157.
63. Ma J, Shi Y, Wang Z, Yue J (2016) On Wiener polarity index of bicyclic networks. *Sci Rep* 6: 19066. doi: [10.1038/srep19066](https://doi.org/10.1038/srep19066) PMID: [26750820](https://pubmed.ncbi.nlm.nih.gov/26750820/)
64. Behmaram A, Yousefi-Azari H, Ashrafi AR (2012) Wiener polarity index of fullerenes and hexagonal systems. *Appl Math Lett* 25: 1510–1513. doi: [10.1016/j.aml.2012.01.006](https://doi.org/10.1016/j.aml.2012.01.006)
65. Hua H, Das KC (2016) On the Wiener polarity index of graphs. *Appl Math Comput* 280: 162–167. doi: [10.1016/j.amc.2016.01.043](https://doi.org/10.1016/j.amc.2016.01.043)
66. Deng H (2010) The wiener polarity index of molecular graphs of alkanes with a given number of methyl groups. *J Serb Chem Soc* 75: 1405–1412. doi: [10.2298/JSC100320114D](https://doi.org/10.2298/JSC100320114D)

67. Liu M, Liu B (2011) On the Wiener polarity index. *MATCH Commun Math Comput Chem* 66: 293–304.
68. Liu M, Liu B (2013) A Survey on recent results of variable Wiener index. *MATCH Commun Math Comput Chem* 69: 491–520.
69. Ma J, Shi Y, Yue J (2014) The Wiener polarity index of graph products. *Ars Combin* 116: 235–244.
70. Zhang Y, Hu Y (2016) The Nordhaus-Gaddum-type inequality for the Wiener polarity index. *Appl Math Comput* 273: 880–884.
71. Chen M, Wang L, Sun S, Wang J, Xia CY (2016) Evolution of cooperation in the spatial public goods game with adaptive reputation assortment. *Physics Letters A* 380(1): 40–47. doi: [10.1016/j.physleta.2015.09.047](https://doi.org/10.1016/j.physleta.2015.09.047)
72. Xia CY, Meloni S, Moreno Y (2012) Effects of environment knowledge on agglomeration and cooperation in spatial public goods games. *Advances in Complex Systems* 15 (supp01): 1250056. doi: [10.1142/S0219525912500567](https://doi.org/10.1142/S0219525912500567)
73. Xia CY, Miao Q, Wang J, Ding S (2014) Evolution of cooperation in the traveler's dilemma game on two coupled lattices. *Appl Math Comput* 246: 389–398. doi: [10.1016/j.amc.2014.08.006](https://doi.org/10.1016/j.amc.2014.08.006)
74. Feng L, Yu G, Xu k, Jiang Z (2014) A note on the Kirchhoff index of bicyclic graphs. *Ars Comb* 114: 33–40.
75. Yu G, Feng L, Ilić A (2011) On the eccentric distance sum of trees and unicyclic graphs. *J Math Anal Appl* 375: 934–944. doi: [10.1016/j.jmaa.2010.08.054](https://doi.org/10.1016/j.jmaa.2010.08.054)
76. Yu G, Feng L, Wang Q (2013) Bicyclic graphs with small positive index of inertia. *Linear Algebra Appl* 438: 2036–2045. doi: [10.1016/j.laa.2012.09.031](https://doi.org/10.1016/j.laa.2012.09.031)
77. Yu G, Liu X, Qu H (2017) Singularity of Hermitian (quasi-)Laplacian matrix of mixed graphs. *Appl Math Comput* 293: 287–292. doi: [10.1016/j.amc.2016.08.032](https://doi.org/10.1016/j.amc.2016.08.032)