DISCRETE MATHEMATICS AND ITS APPLICATIONS

QUANTITATIVE GRAPH THEORY

Mathematical Foundations and Applications

Edited by

Matthias Dehmer
Frank Emmert-Streib

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Chapter 9

Wiener Index of Line Graphs

Martin Knor and Riste Škrekovski

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9.1 Introduction

We consider the molecular descriptor Wiener index, W, of graphs and their line graphs. This index plays a crucial role in organic chemistry. It was studied by chemists decades before it attracted attention of mathematicians. In fact, it was studied long time before the branch of discrete mathematics, which is now known as graph theory, was born. Nowadays, there are many indices known used to describe the molecules.

In this chapter, we first introduce the concept of topological indices and list some of them. Next, in the third section, we focus on the Wiener index and expose some of its properties. Furthermore, we compare the values $W(G)$ and $W(L(G))$, in particular when they are equal for G being in various classes of graphs. In addition, we expose some bounds of the Wiener index of the line graph in terms of the Gutman index of the original graph. In the next section, we consider the equality $W(G) = W(L(G))$ for graphs with large girth. Finally, we consider the same equality for trees but for higher iterations of line graphs, $W(T) = W^i(L(T))$. The sixth section is dedicated to the case $i = 2$. In the seventh section, we show that a solution of

$$W(L^i(T)) = W(T) \quad (i \geq 3)$$

exists only for $i = 3$, and it is one particular class of trees, all homeomorphic to the letter H. The smallest such tree has 388 vertices.

9.2 Indices in Chemical Graph Theory

Graphs and networks can be described in quantitative terms using different measures or indices. They function as a universal language to describe the chemical structure of molecules, the chemical reaction networks, ecosystems, financial markets, the World Wide Web, and social networks. In chemical graph theory, we refer to these measures as topological indices or molecular descriptors.

Considering chemical structures as graphs is an important methodology for understanding chemical structures and reactivity. In molecular graphs, the atoms are represented by vertices and the bonds by edges. In chemistry, the degree of a vertex is called its valence. Double bonds or lone-pair electrons can be represented by multiple edges and self loops [55,57]. In this way, graph theory provides simple rules by which chemists may obtain qualitative predictions about the structure and reactivity of various chemical compounds [59].

Topological indices are numerical invariants of molecular graphs, and they may be used as numerical descriptors to derive quantitative structure–property relationships (QSPR) or quantitative structure–activity relationships (QSAR). Both QSAR and QSPR are showing the tendency to predict the properties of a compound based on its molecule structure.

When talking about topological indices (as quantitative graph measures), one can distinguish them in groups, for example,

- Distance based (Wiener index, etc.),
- Degree based (Zagreb indices, etc.),
- Graph spectra based (Estrada index, etc.),
- Information-theoretic indices based on Shannon's entropy.

The oldest topological index related to molecular branching is the Wiener index [61], which was introduced in 1947 as the path number. The same quantity has been studied and referred to in mathematics as the gross status [41], the distance of graphs [24], and the transmission [60]. The *Wiener* index of a graph G, denoted by $W(G)$, is the sum of distances between all (unordered) pairs of vertices of G

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v). \tag{9.1}$$

Though the Wiener index is the most common topological characteristic of a graph, nowadays, we know over 200 indices, and we devote this section to listing a few of them.

For an edge $e = ij$, let $n_e(i)$ be the number of vertices of G being closer to i than to j and $n_e(j)$ be the number of vertices of G lying closer to j than to i. The *Szeged* index of a graph G is defined by

$$Sz(G) = \sum_{e=ij \in E(G)} n_e(i) n_e(j).$$

This invariant was introduced by Gutman [30] during a stay at the Attila Jozsef University in Szeged, and he named it after this place.

The first Zagreb index M_1 and the second Zagreb index M_2 were defined in [39] as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v),$$

where $d(u)$ and $d(v)$ denote the degree of u and v. Zagreb indices are used by various researchers in their QSPR and QSAR studies [12], as well as in molecular complexity [54]. In 1975, the *Randić* index $R(G)$ of a graph G was defined as

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}.$$

It has been proved to be suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons [56].

In 1989, led by the idea of characterizing the alkanes, Schultz defined a new index that is degree and distance based [58]. Recently, this index is known as *Schultz index* (*of first kind*), and it is defined by

$$S(G) = \sum_{\{u,v\} \subseteq V(G)} (d(u) + d(v))\, d(u,v).$$

Inspired by the Schultz index, Gutman [31] back in 1994 introduced a new index,

$$\mathrm{Gut}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u)d(v)d(u,v),$$

and named it the *Schultz index of second kind*. Nowadays, this index is also known as the *Gutman* index.

All of the aforementioned topological indices are degree- and distance-based molecular descriptors, but there are also indices of a different kind. The *Hosoya* index, also known as the Z index, of a graph describes the total number of matchings within the graph. This index was introduced by Hosoya in [42] and is often used for investigations of organic compounds [44]. A high correlation exists between the Hosoya index and the boiling points of acyclic alkanes.

The *Estrada* index was introduced in 2000 as a measure of the degree of a protein folding [25]. Later, the Estrada index was used also to measure the centrality of other complex networks, such as communication, social, and metabolic networks [26,27]. This index includes the eigenvalues λ_i, $i = 1, \ldots, n$, of the adjacency matrix of a graph G and is defined as

$$\mathrm{EE}(G) = \sum_{i=1}^{n} e^{\lambda_i}.$$

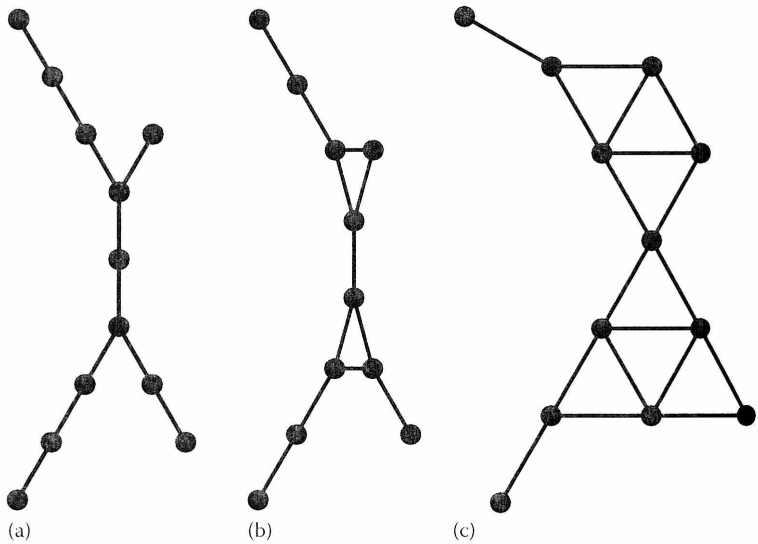

FIGURE 9.1: (a) Graph, (b) its line graph, and (c) its second iterated line graph.

For the entropy-based indices, see the books Bonchev [6] and Dehmer [9] and the articles [10,11] as well.

Since we focus on line graphs in this chapter, let us recall the definition of (iterated) line graphs. Let G be a graph. Its *line graph*, $L(G)$, has vertex set identical with the set of edges of G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G (see Figure 9.1 for illustration). *Iterated* line graphs are defined inductively as follows:

$$L^i(G) = \begin{cases} G & \text{if } i = 0, \\ L(L^{i-1}(G)) & \text{if } i > 0. \end{cases}$$

We recall that although there is a characterization of line graphs by forbidden subgraphs [2], there does not exist a similar characterization for i-iterated line graphs for $i \geq 2$.

9.3 Wiener Index

At first, the Wiener index was used for predicting the boiling point of paraffin [59], but later, strong correlation between the Wiener index and the chemical properties of a compound was found. Nowadays, this index is a tool used for preliminary screening of drug molecules [1]. The Wiener index also predicts binding energy of protein–ligand complex at a preliminary stage.

Besides introducing (new) index, Wiener also stated a theorem that shows how the Wiener index of a tree can be decomposed into easily calculable edge–contributions. Denote by $N_2(F)$ the sum over all pairs of components of the product of the number of vertices of two components of a forest F, that is,

$$N_2(F) = \sum_{1 \le i < j \le p} n(T_i)\, n(T_j),$$

where $T_1, T_2, \ldots, T_p$ is the set of components of F. If $p = 1$, that is, if F is connected, then $N_2(F) = 0$.

Theorem 9.3.1 *[61] For a tree T, the following holds:*

$$W(T) = \sum_{e \in E(T)} N_2(T - e). \tag{9.2}$$

Proof. Notice that in a tree any two vertices are connected by a unique path, which is the shortest one. So, an edge $e = ij$ contributes 1 to $W(T)$ for each pair of vertices for which the unique path between them contains e. And, this is a case when i and j are in distinct components of $T - e$. As the number of such paths is $N_2(F - e)$, the proof follows. □

As T is a tree, for every edge $e = ij$ of T, the forest $T - e$ is composed of two components, one of size $n_e(i)$ and the other of size $n_e(j)$, which gives $N_2(T - e) = n_e(i)n_e(j)$. Thus, one can restate (9.2) as

$$W(T) = \sum_{e = ij \in E(T)} n_e(i)n_e(j). \tag{9.3}$$

So the Szeged index and the Wiener index coincide on trees. In fact, the Szeged index was defined from (9.3) by relaxing the condition that the graph is a tree.

In analogy to the classical Theorem 9.3.1, we have the following vertex version (see [38]):

Theorem 9.3.2 *Let T be a tree on n vertices. Then,*

$$W(T) = \sum_{v \in V(T)} N_2(T - v) + \binom{n}{2}. \tag{9.4}$$

A theorem given by Doyle and Graver [22] is of a similar kind. In order to state it, denote by $N_3(F)$ the sum over all triplets of components of the product of the number of vertices of three components of a forest F, that is,

$$N_3(F) = \sum_{1 \le i < j < k \le p} n(T_i)\, n(T_j)\, n(T_k).$$

Note that if $p = 1$ or $p = 2$, then $N_3(F) = 0$. This theorem claims the following.

Theorem 9.3.3 (Doyle and Graver) *Let T be a tree on n vertices. Then,*

$$W(T) = \binom{n+1}{3} - \sum_{v \in V(T)} N_3(T - v).$$

The Wiener index is also closely related to other quantities. For example, in computer science, the average distance $\mu(G)$ is used, where

$$\mu(G) = \frac{W(G)}{\binom{|V(G)|}{2}}.$$

It is important to know the average distance traversed by a message in the network. Networks with small $\mu(G)$ are related to *small worlds*.

In the theory of social networks, the Wiener index is closely related to the betweenness centrality of a vertex that quantifies the number of times a vertex lays on a shortest path between two other vertices. More precisely, the *betweenness centrality* $B(x)$ of a vertex $x \in V(G)$ is the sum of the fraction of all-pairs shortest paths that pass through x, that is,

$$B(x) = \sum_{\substack{u,v \in V(G) \\ u \neq v \neq x}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}}, \tag{9.5}$$

where

$\sigma_{u,v}$ denotes the total number of shortest (u, v) paths in G
$\sigma_{u,v}(x)$ represents the number of shortest (u, v) paths passing through the vertex x.

This is one of the most important centrality indices. It was introduced by Anthonisse [3] and popularized later by Freeman [28].

The following result tells that the sum of the betweenness centrality of all vertices of a graph is related to its Wiener index. Moreover, it is a generalization of (9.4) to connected graphs with cycles [38].

Theorem 9.3.4 *For any connected graph G, the following holds:*

$$W(G) = \sum_{v \in V(G)} B(v) + \binom{n}{2}.$$

Since for any pair of vertices in a tree the shortest path between them is unique, the Wiener index of a tree is much easier to compute than that of an arbitrary graph. Furthermore, it is easy to see that for trees on n vertices, the maximal Wiener index is obtained for the path P_n, and

$$W(P_n) = \binom{n+1}{3}.$$

On the other hand, the tree with minimal Wiener index is the star S_n, and

$$W(S_n) = (n-1)^2.$$

Thus, for every tree T on n vertices, we have

$$(n-1)^2 \le W(T) \le \binom{n+1}{3}.$$

As the distance between any two distinct vertices is at least one, we have that K_n has the smallest Wiener index between all graph on n vertices. So for any connected graph G on n vertices, it holds:

$$\binom{n}{2} \le W(G) \le \binom{n+1}{3}.$$

Among the 2-connected graphs on n vertices (or even more, among the graphs of minimum degree 2), the n-cycle has the largest Wiener index

$$W(C_n) = \begin{cases} \dfrac{n^3}{8} & \text{if } n \text{ is even,} \\ \dfrac{n^3 - n}{8} & \text{if } n \text{ is odd.} \end{cases}$$

The Wiener index is easy to obtain for some classes of graphs. For graphs G and H, the Wiener index of their Cartesian product $G \square H$ is

$$W(G \square H) = |n(G)|^2 \cdot W(H) + |n(H)|^2 \cdot W(G),$$

see [29]. From this result follows a simple formula for the Wiener index of hypercubes Q_n

$$W(Q_n) = n2^{2(n-1)}.$$

We conclude this section with an interesting connection between the Wiener index and Laplacian spectrum of a tree.

Theorem 9.3.5 *Let T be a tree with Laplacian eigenvalues $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_{n-1} > \lambda_n = 0$. Then,*

$$W(T) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i}.$$

In 1988, Hosoya [43] introduced

$$H(G, x) = \sum_{k=1}^{l} d(G, k) x^k,$$

where
  G is a graph
  $d(G, k)$ is the number of pairs of vertices in the graph G at distance k.

Originally, this polynomial was named Wiener polynomial, but later, it was renamed into Hosoya polynomial. The first derivative of $H(G,x)$ for $x = 1$ is equal to the Wiener index of the graph G. This property of the Hosoya polynomial gives an alternative way of calculating the Wiener index and in a way makes the Hosoya polynomial a generalization of $W(G)$. Higher derivatives of Hosoya polynomial are also used as molecular descriptors (the hyper-Wiener index, e.g., is one half of the second derivative of $H(G,x)$ for $x = 1$).

For further details and results on the Wiener index, see [15,16,23,37,40] and the references cited therein.

9.4 Wiener Index of Graphs and Their Line Graphs

The concept of line graphs and iterated line graphs in chemical graph theory is introduced in order to study the molecule complexity. The number of edges in the line graph of the molecular graph is a measure of the branching, and then the iterated line graphs are used to find complete ordering of the molecules [5]. See [33,36] for some more applications in physical chemistry.

On the other hand, mathematicians started to study the connection between $W(G)$ and $W(L(G))$. In particular, they focused on graphs G satisfying

$$W(L(G)) = W(G). \tag{9.6}$$

Although it is not clear on which graph parameters or structural properties the difference $W(L(G)) - W(G)$ depends, the problem of characterizing graphs G with $W(L(G)) = W(G)$ is interesting, and it seems to be rather difficult.

In this section, we summarize some results on this issue, for more results on the topic, see [8,18,19,33,35]. Let us remark that in the literature, one easily encounters the term *edge-Wiener index* of G, which is actually the Wiener index of the line graph, sometimes in addition shifted by $\binom{n}{2}$, see [45].

The following remark of Buckley [7] is a pioneering work in this area.

Theorem 9.4.1 (Buckley, 1981) *For every tree T, $W(L(T)) = W(T) - \binom{n}{2}$.*

Proof. Let u, v be two distinct vertices of T. On their shortest (and unique) path in T, let e_u be the edge incident with u and e_v the edge incident with v. Notice that e_u and e_v coincide when u and v are adjacent. There is an obvious one-to-one correspondence between the pairs of distinct vertices u, v and their corresponding pairs of edges e_u, e_v. As there are $\binom{n}{2}$ pairs of vertices, and for each such pair u, v, it holds $d_{L(T)}(e_u, e_v) = d_T(u, v) - 1$, we conclude the statement of the theorem. □

In particular, the aforementioned result tells that regarding the acyclic graphs, the Wiener index of a line graph is strictly smaller than the Wiener index of the original graph. An interesting generalization of this was given by Gutman [32]:

Theorem 9.4.2 *If G is a connected graph with n vertices and m edges, then*

$$W(L(G)) \geq W(G) - n(n-1) + \frac{1}{2}m(m+1).$$

In addition, regarding Theorem 9.4.1, Gutman and Pavlović [35] showed that the Wiener index of the line graph is smaller than the Wiener index of the original graph even if we allow just one cycle in the graph.

Theorem 9.4.3 *If G is a connected unicyclic graph with n vertices, then $W(L(G)) \leq W(G)$, with equality if and only if G is a cycle of length n.*

In connected bicyclic graphs, all the three cases $W(L(G)) < W(G)$, $W(L(G)) = W(G)$, and $W(L(G)) > W(G)$ occur [35]. It is known that the smallest bicyclic graph with the property $W(L(G)) = W(G)$ has nine vertices and it is unique. There are already 26 ten-vertex bicyclic graphs with the same property [34].

The following result tells us that in most cases (9.6) does not hold for graphs of minimum degree at least 2.

Theorem 9.4.4 *Let G be a connected graph with $\delta(G) \geq 2$. Then,*

$$W(L(G)) \geq W(G).$$

Moreover, the equality holds only for cycles.

This was proved independently and simultaneously in [7,62]. In [7], a direct proof of this result is given. On the other hand, Wu [62] obtained it as a corollary from his interesting result on the bounds of the Wiener index of line graphs in terms of the Gutman index:

Theorem 9.4.5 *Let G be a connected graph of size m. Then, it holds*

$$\frac{1}{4}(\mathrm{Gut}(G) - m) \leq W(L(G)) \leq \frac{1}{4}(\mathrm{Gut}(G) - m) + \binom{m}{2}.$$

Moreover, the lower bound is attained if and only if G is a tree.

Let $\kappa_i(G)$ denote the number of i-cliques in a graph G. In [48], the lower bound of the aforementioned theorem is improved in the following way.

Theorem 9.4.6 *Let G be a connected graph. Then,*

$$W(L(G)) \geq \frac{1}{4}\mathrm{Gut}(G) - \frac{1}{4}|E(G)| + \frac{3}{4}\kappa_3(G) + 3\kappa_4(G) \tag{9.7}$$

with the equality in (9.7) if and only if G is a tree or a complete graph.

The aforementioned theorem implies the following interesting corollary.

Corollary 9.4.1 *Let G be a connected graph of minimal degree $\delta \geq 2$. Then,*

$$W(L(G)) \geq \frac{\delta^2}{4} W(G) - \frac{1}{4}|E(G)| \geq \frac{\delta^2 - 1}{4} W(G).$$

Proof. Note that

$$\mathrm{Gut}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u)d(v)d(u,v) \geq \sum_{\{u,v\} \subseteq V(G)} \delta^2 d(u,v) = \delta^2 W(G).$$

Now, since $\delta \geq 2$, the graph G is not a tree, and so Theorem 9.4.6 implies the first inequality in the corollary. The second inequality then follows, if one observes that, since every pair of adjacent vertices contributes exactly 1 to the Wiener index of the graph (while the nonadjacent ones contribute even more), we have that $|E(G)| \leq W(G)$. □

We expect that Corollary 9.4.1 can be improved to $W(L(G)) \geq \frac{\delta^2}{4} W(G)$, with equality holding for cycles, which would correspond to the result of Wu for $\delta = 2$.

9.5 Graphs with Large Girth

A connected graph G is isomorphic to $L(G)$ if and only if G is a cycle. Thus, the cycles provide a trivial infinite family of graphs for which $W(G) = W(L(G))$. In addition, for every positive number g, there exists a graph G with girth g for which $W(G) = W(L(G))$.

Dobrynin and Mel'nikov [17] have constructed infinite family of graphs of girths 3 and 4 with the property $W(G) = W(L(G))$ and stated the following problem.

Problem 9.5.1 (Dobrynin and Mel'nikov) *Is it true that for every integer $g \geq 5$ there exists a graph $G \neq C_g$ of girth g, for which $W(G) = W(L(G))$?*

The aforementioned problem was solved by Dobrynin [14] by considering the following construction. Let $G_g(d,s,r)$ be a graph of girth g constructed from a path P_d by

1. Identifying a vertex of a distinct copy of the g-cycle C_g with each of the end vertices of P_d
2. Identifying the center of disjoint copies of the S_{s+1}-star with one end vertex and of the S_{r+1}-star with the other end vertex of P_d

Observe that G is a bicyclic graph of girth g with $2g + d + s + r - 2$ vertices (see Figure 9.2). In [14], the following result is shown.

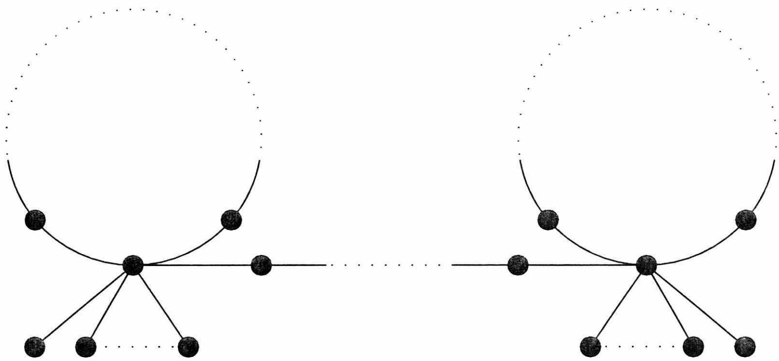

FIGURE 9.2: The graph $G_g(d, r, s)$ with $W(G_g(d, r, s)) = W(L(G_g(d, r, s)))$.

Theorem 9.5.1 (Dobrynin) *The Wiener indices of $G_g(d, s, r)$ and $L(G_g(d, s, r))$ coincide provided that the graph parameters satisfy the following relations:*

(*a*) *For every even $g \geq 6$,*

$$d = (g^2 - 6g + 4)/4, \quad s = (g^2 - 6g + 8)/8, \quad r = (g^2 - 6g + 16)/8.$$

(*b*) *For every odd $g \geq 9$,*

$$d = (g^2 - 8g + 3)/4, \quad s = (g^2 - 8g + 15)/8, \quad r = (g^2 - 8g + 23)/8.$$

Theorem 9.5.1 overlooks the values $g = 5$ and $g = 7$. For $g = 5$, see the graph G_5 on Figure 9.3. Both G_5 and its line graph $L(G_5)$ have Wiener indices 288. For $g = 7$, the graph $G_7 = G_7(6, 4, 5)$ satisfies $W(G_7) = W(L(G_7)) = 1698$.

The authors of [7] showed that for infinitely many girths, there exist infinitely many solutions of Problem 9.5.1.

Theorem 9.5.2 *For every positive integer g_0, there exists $g \geq g_0$ such that there are infinitely many graphs G of girth g satisfying $W(G) = W(L(G))$.*

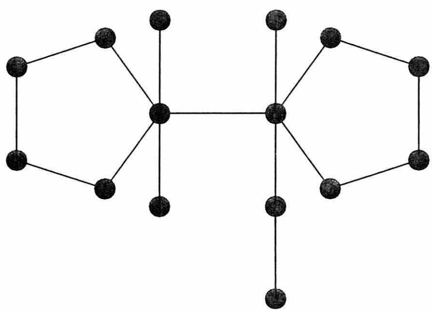

FIGURE 9.3: The graph G_5 of girth 5 with $W(G_5) = W(L(G_5))$.

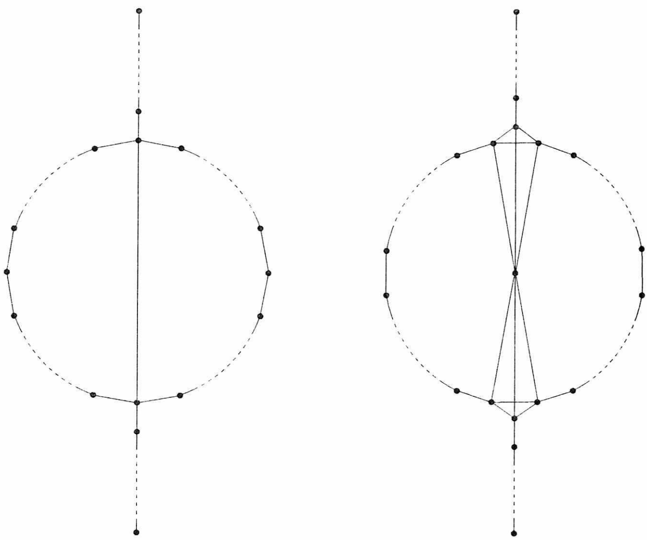

FIGURE 9.4: Graphs $\Phi(k,p,q)$ and $L(\Phi(k,p,q))$.

The aforementioned result encourages the authors of [7] to state the following conjecture. Notice that it is true for girths 3 and 4, see [17].

Conjecture 9.5.1 *For every integer $g \geq 3$, there exist infinitely many graphs G of girth g satisfying $W(G) = W(L(G))$.*

In what follows, we give a sketch of the proof of Theorem 9.5.2. For positive integers k,p,q, we define the graph $\Phi(k,p,q)$ as follows (see Figure 9.4 for an illustration). The graph $\Phi(k,p,q)$ is simple and composed of two cycles, $C_1 = u_1u_2\dots u_{2k+1}$ and $C_2 = v_1v_2\dots v_{2k+1}$, and two paths $P_p = x_1x_2\dots x_p$ and $P_q = y_1y_2\dots y_q$ such that all the vertices are distinct except for $v_1 = u_1 = x_1$ and $y_1 = v_{2k+1} = u_{2k+1}$.

We are now interested in computing the difference $W(L(\Phi(k,p,q))) - W(\Phi(k,p,q))$, which is used in the proof of Theorem 9.5.4. The proof is straightforward and rather technical.

Theorem 9.5.3 *For integers, $k,p,q \geq 1$, let $G = \Phi(k,p,q)$ with girth $g = 2k+1$. Then,*

$$W(L(G)) - W(G) = \frac{1}{2}(g^2 + (p-q)^2 + 5(p+q-3) - 2g(p+q-3)).$$

Theorem 9.5.3 implies the following result:

Theorem 9.5.4 *For every nonnegative integer h, there exist infinitely many graphs G of girth $g = h^2 + h + 9$ with $W(L(G)) = W(G)$.*

Theorem 9.5.2 is an immediate corollary of Theorem 9.5.4. For every positive integer g_0, we can choose a nonnegative integer h such that $g = h^2 + h + 9 \geq g_0$. By Theorem 9.5.4, there are infinitely many graphs G of girth g with $W(L(G)) = W(G)$.

9.6 Second Line Graph Iteration

The graph $L^2(G) = L(L(G))$ is also called the *quadratic line graph* of G. As mentioned earlier, for nontrivial tree T, we cannot have $W(L(T)) = W(T)$ although there are graphs G such that $W(L(G)) = W(G)$. For quadratic line graphs, we can have

$$W(L^2(T)) = W(T), \tag{9.8}$$

even if T is a tree (see [13,20,21]). Obviously, the simplest trees are such which have a unique vertex of degree greater than 2. Such trees are called *generalized stars*. More precisely, *generalized t-star* is a tree obtained from the star $K_{1,t}$, $t \geq 3$, by replacing all its edges by paths of positive lengths. In [17], we have the following theorem.

Theorem 9.6.1 *Let S be a generalized t-star with q edges and branches of length $k_1, k_2, \ldots, k_t$. Then,*

$$W(L^2(S)) = W(S) + \frac{1}{2}\binom{t-1}{2}\left(\sum_{i=1}^{t} k_i^2 + q\right) - q^2 + 6\binom{t}{4}. \tag{9.9}$$

Based on this theorem, it is proved in [17] that $W(L^2(S)) < W(S)$ if S is a generalized 3-star, and $W(L^2(S)) > W(S)$ if S is a generalized t-star where $t \geq 7$. Thus, property (9.8) can hold for generalized t-stars only when $t \in \{4, 5, 6\}$. In [17], for every $t \in \{4, 5, 6\}$, several generalized t-stars with property (9.8) are found. The smallest generalized t-stars with property (9.8) are listed in Table 9.1 (see also [17]).

From Table 9.1, one can expect that it might be easier to find generalized t-stars with property (9.8) when $t \in \{5, 6\}$ than in the case $t = 4$. Indeed, in [17], the authors

TABLE 9.1: Smallest Generalized t-Stars with the Property (9.8)

t	q	k_1	k_2	k_3	k_4	k_5	k_6	q	k_1	k_2	k_3	k_4	k_5	k_6
4	27	1	2	3	21	—	—	90	3	7	8	72	—	—
	42	1	2	6	33	—	—	102	2	3	16	81	—	—
	69	2	6	6	55	—	—	105	4	5	12	84	—	—
	72	1	3	11	57	—	—	105	2	9	10	84	—	—
	90	4	5	9	72	—	—	111	4	9	9	89	—	—
5	18	2	3	3	3	7	—	30	4	4	4	4	14	—
	24	2	3	3	6	10	—	30	3	3	3	8	13	—
	24	2	2	5	5	10	—	30	1	4	5	7	13	—
	24	1	4	4	5	10	—	36	4	4	4	7	17	—
	24	1	2	6	6	9	—	36	3	4	6	6	17	—
6	50	7	7	7	8	10	11	60	7	8	8	10	13	14
	50	6	7	8	9	9	11	60	6	8	9	11	12	14
	50	5	8	9	9	9	10	60	6	7	10	12	12	13
	60	8	8	8	9	12	15	60	5	10	10	10	11	14
	60	6	9	10	10	10	15	60	5	8	11	12	12	12

TABLE 9.2: Infinite Families of Generalized t-Stars, $t \in \{5, 6\}$, with the Property (9.8)

t	k_1	k_2	k_3	k_4	k_5	k_6
5	1	2	$2k^2 - k + 5$	$2k^2 - k + 5$	$2k^2 + 2k + 5$	—
	1	2	$2k^2 - 2k + 5$	$2k^2 + k + 5$	$2k^2 + k + 5$	—
	1	2	$2k^2 + 6$	$2k^2 + 3k + 6$	$2k^2 + 3k + 9$	—
6	3	$4k^2 + 33$	$4k^2 - k + 36$	$4k^2 - k + 36$	$4k^2 + k + 36$	$4k^2 + k + 36$

TABLE 9.3: Infinite Families of Generalized 4-Stars with the Property (9.8)

k_1	k_2	k_3	k_4
$a_1(k)$	$a_1(k+1)$	$4(k_1 + k_2) - 3$	$4(k_1 + k_2 + k_3) - 3$
1	$a_2(k)$	$a_2(k+1)$	$4(k_1 + k_2 + k_3) - 3$
2	$a_3(k)$	$a_3(k+1)$	$4(k_1 + k_2 + k_3) - 3$
3	$a_4(k)$	$a_4(k+1)$	$4(k_1 + k_2 + k_3) - 3$
4	$a_5(k)$	$a_5(k+1)$	$4(k_1 + k_2 + k_3) - 3$
5	$a_6(k)$	$a_6(k+1)$	$4(k_1 + k_2 + k_3) - 3$
6	$a_7(k)$	$a_7(k+1)$	$4(k_1 + k_2 + k_3) - 3$
1	2	$a_8(k)$	$a_8(k+1)$
4	5	$a_9(k)$	$a_9(k+1)$
4	5	$a_{10}(k)$	$a_{10}(k+1)$

found infinite families of these generalized t-stars for $t \in \{5, 6\}$. They found three infinite families for $t = 5$ and one for $t = 6$, see Table 9.2, where k is nonnegative integer. Observe that the first two infinite families of generalized 5-stars can be regarded as one provided that $k \in \mathbb{Z}$ only.

The problem of existence of an analogous infinite family of generalized 4-stars is left open in [17]. This problem is solved in [53], where several infinite families of generalized 4-stars with the property (9.8) are constructed. The constructions are grouped into three classes, and there is an infinite number of families in two of these three classes. Some of these constructions, grouped into families, are listed in Table 9.3, where $k \in \mathbb{Z}$. As regards the values of sequences $a_1, \ldots, a_{10}$, we have

$$a_1(j) = \frac{1}{4}\left(5 + \sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{4}\left(5 - \sqrt{3}\right)\left(2 + \sqrt{3}\right)^j + \frac{3}{2}$$

$$a_2(j) = \frac{1}{12}\left(15 + 3\sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{12}\left(15 - 3\sqrt{3}\right)\left(2 + \sqrt{3}\right)^j - \frac{1}{2}$$

$$a_3(j) = \frac{1}{12}\left(21 + 3\sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{12}\left(21 - 3\sqrt{3}\right)\left(2 + \sqrt{3}\right)^j - \frac{5}{2}$$

$$a_4(j) = \frac{1}{12}\left(33 + 9\sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{12}\left(33 - 9\sqrt{3}\right)\left(2 + \sqrt{3}\right)^j - \frac{9}{2}$$

$$a_5(j) = \frac{1}{12}\left(69 - 33\sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{12}\left(69 + 33\sqrt{3}\right)\left(2 + \sqrt{3}\right)^j - \frac{13}{2}$$

$$a_6(j) = \frac{1}{12}\left(75 - 33\sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{12}\left(75 + 33\sqrt{3}\right)\left(2 + \sqrt{3}\right)^j - \frac{17}{2}$$

$$a_7(j) = \frac{1}{12}\left(69 + 21\sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{12}\left(69 - 21\sqrt{3}\right)\left(2 + \sqrt{3}\right)^j - \frac{21}{2}$$

$$a_8(j) = \frac{1}{12}\left(45 - 21\sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{12}\left(45 + 21\sqrt{3}\right)\left(2 + \sqrt{3}\right)^j - \frac{9}{2}$$

$$a_9(j) = \frac{1}{12}\left(153 - 75\sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{12}\left(153 + 75\sqrt{3}\right)\left(2 + \sqrt{3}\right)^j - \frac{33}{2}$$

$$a_{10}(j) = \frac{1}{12}\left(297 - 165\sqrt{3}\right)\left(2 - \sqrt{3}\right)^j + \frac{1}{12}\left(297 + 165\sqrt{3}\right)\left(2 + \sqrt{3}\right)^j - \frac{33}{2}.$$

These results suggest the following conjecture:

Conjecture 9.6.1 *Let T be a nontrivial tree such that $W\left(L^2(T)\right) = W(T)$. Then, there is an infinite family of trees T' homeomorphic to T, such that $W(L^2(T')) = W(T')$.*

Of course, more interesting is the question which types of trees satisfy (9.8). Perhaps such trees do not have many vertices of degree at least 3. Let $\mathcal{T}$ be a class of trees that have no vertex of degree two, and such that $T \in \mathcal{T}$ if and only if there exists a tree T' homeomorphic to T, and such that $W\left(L^2(T')\right) = W(T')$. (Recall that graphs G_1 and G_2 are homeomorphic if and only if the graphs obtained from them by repeatedly removing a vertex of degree 2, and making its two neighbors adjacent, are isomorphic.)

Problem 9.6.1 *Characterize the trees in $\mathcal{T}$. In particular, prove that $\mathcal{T}$ is finite.*

By the aforementioned results, among the stars, only $K_{1,4}$, $K_{1,5}$, and $K_{1,6}$ are in $\mathcal{T}$. We expect that no tree in $\mathcal{T}$ has a vertex of degree exceeding 6. Based on our experience, we also expect that there is a constant c such that no tree in $\mathcal{T}$ has more than c vertices of degree at least 3. Consequently, we believe that the set $\mathcal{T}$ is finite.

9.7 Higher Line Graph Iterations

As we have seen, there is no nontrivial tree for which $W(L(T)) = W(T)$ and there are many trees T, satisfying $W(L^2(T)) = W(T)$. However, it is not easy to find a tree T and $i \geq 3$ such that $W(L^i(T)) = W(T)$. In [15], the following problem was posed.

Problem 9.7.1 *[15] Is there any tree T satisfying equality $W(L^i(T)) = W(T)$ for some $i \geq 3$?*

Observe that if T is a trivial tree, then $W(L^i(T)) = W(T)$ for every $i \geq 1$, although here the graph $L^i(T)$ is empty. The real question is, of course, if there is a nontrivial tree T and $i \geq 3$ such that $W(L^i(T)) = W(T)$. The same question appeared 4 years later in [17] as a conjecture. The authors expressed their belief that the problem has no nontrivial solution.

Conjecture 9.7.1 (Dobrynin, Entringer) *There is no tree T satisfying equality $W(T) = W(L^i(T))$ for any $i \geq 3$.*

In a series of papers [4,47,49–52], Conjecture 9.7.1 was disproved. In fact, all solutions of Problem 9.7.1 were found. The smallest tree disproving Conjecture 9.7.1 has 388 vertices (see the remark below Theorem 9.7.7) and this tree is unique. If we take in mind that there are approximately $7.5 \cdot 10^{175}$ nonisomorphic trees on 388 vertices while the number of atoms in the entire universe is estimated to be only within the range of 10^{78} to 10^{82}, then to find *a needle in a haystack* is a trivially easy job compared to finding a counterexample when using only the brute force of (arbitrarily many) real computers.

A function $f : \{0, 1, \ldots\} \rightarrow \mathbb{R}$ is *convex* if $f(i) + f(i+2) \geq 2f(i+1)$ for every $i \geq 0$. If the inequality is strict, then f is *strictly convex*. In [50], it is proved that for every connected graph G, the function $f_G(i) = W(L^i(G))$ is convex in variable i. Moreover, $f_G(i)$ is strictly convex if G is distinct from a path, a cycle, and the claw $K_{1,3}$. The following result is a straightforward consequence of this fact.

Theorem 9.7.1 *Let T be a tree such that $W(L^3(T)) > W(T)$. Then, for every $i \geq 3$, the inequality $W(L^i(T)) > W(T)$ holds.*

Let G be a graph. A *pendant path* (or a *ray* for short) R in G is a (directed) path; the first vertex of which has degree at least 3, its last vertex has degree 1, and all of its internal vertices (if any exist) have degree 2 in G. Observe that if R has length t, $t \geq 2$, then the edges of R correspond to vertices of a ray $L(R)$ in $L(G)$ of length $t-1$. In [50], we have the following theorem.

Theorem 9.7.2 *Let T be a tree distinct from a path and the claw $K_{1,3}$ such that all of its rays have length 1. Then, $W(L^3(T)) > W(T)$.*

In [49], this statement was extended to trees with arbitrarily long rays. Denote by H a tree on six vertices, two of which have degree 3 and the remaining four have degree 1. That is, H is the graph which *looks* like the letter H. The main result of [49] is the following theorem.

Theorem 9.7.3 *Let T be a tree not homeomorphic to a path, claw $K_{1,3}$, and H. Then, $W(L^3(T)) > W(T)$.*

Combining Theorems 9.7.1 and 9.7.3, we obtain the following consequence, which proves Conjecture 9.7.1 for trees T satisfying the assumption in Theorem 9.7.3.

Theorem 9.7.4 *Let T be a tree not homeomorphic to a path, claw $K_{1,3}$, and H. Then, $W(L^i(T)) > W(T)$ for every $i \geq 3$.*

Since the case when T is a path is trivial (in this case, $W(L^i(T)) < W(T)$ whenever $i \geq 1$, and T has at least two vertices), it remains to consider graphs homeomorphic to the claw $K_{1,3}$ and those homeomorphic to H.

First, consider the case of the claw $K_{1,3}$ itself. Then, $L^i(K_{1,3})$ is a cycle of length 3 for every $i \geq 1$. Since $W(K_{1,3}) = 9$ and the Wiener index of the cycle of length 3 is 3, we have $W(L^i(K_{1,3})) < W(K_{1,3})$ for every $i \geq 1$. For other trees homeomorphic to $K_{1,3}$, the opposite inequality is proved in [52], provided that $i \geq 4$.

Theorem 9.7.5 *Let T be a tree homeomorphic to $K_{1,3}$, such that $T \neq K_{1,3}$. Then, $W(L^i(T)) > W(T)$ for every $i \geq 4$.*

Notice that it was enough to prove the aforementioned theorem for the case $i = 4$, since then the inequalities with higher powers follow from the convexity of $f_G(i) = W(L^i(G))$. Analogous statement for trees homeomorphic to H was proved in [51].

Theorem 9.7.6 *Let T be a tree homeomorphic to H. Then, $W(L^i(T)) > W(T)$ for every $i \geq 4$.*

Consequently, with the exception of paths and the claw $K_{1,3}$, for every tree T, it holds $W(L^i(T)) > W(T)$ whenever $i \geq 4$. We can summarize the results for $i \geq 4$ as follows.

Corollary 9.7.1 *Let T be a tree and $i \geq 4$. Then, the following holds:*

$$\begin{aligned}
&W\left(L^i(T)\right) < W(T) \quad && \textit{if } T \textit{ is the claw } K_{1,3} \textit{ or a path } P_n \textit{ with } n \geq 2;\\
&W\left(L^i(T)\right) = W(T) \quad && \textit{if } T \textit{ is the trivial graph } P_1;\\
&W\left(L^i(T)\right) > W(T) \quad && \textit{otherwise.}
\end{aligned}$$

Hence, Conjecture 9.7.1 is true for $i \geq 4$. However, for $i = 3$, the infinite class of trees described in Theorem 9.7.7 violates Conjecture 9.7.1 (see [47]).

Let $H_{a,b,c}$ be a tree on $a+b+c+4$ vertices, out of which two have degree 3, four have degree 1, and the remaining $a+b+c-2$ vertices have degree 2. The two vertices of degree 3 are connected by a path of length 2. Finally, there are two pendant paths of lengths a and b attached to one vertex of degree 3 and two pendant paths of lengths c and 1 attached to the other vertex of degree 3 (see Figure 9.5 for $H_{3,2,4}$). We have

Theorem 9.7.7 *For every $j, k \in \mathbb{Z}$, define*

$$\begin{aligned}
a &= 128 + 3j^2 + 3k^2 - 3jk + j,\\
b &= 128 + 3j^2 + 3k^2 - 3jk + k,\\
c &= 128 + 3j^2 + 3k^2 - 3jk + j + k.
\end{aligned}$$

Then, $W(L^3(H_{a,b,c})) = W(H_{a,b,c})$.

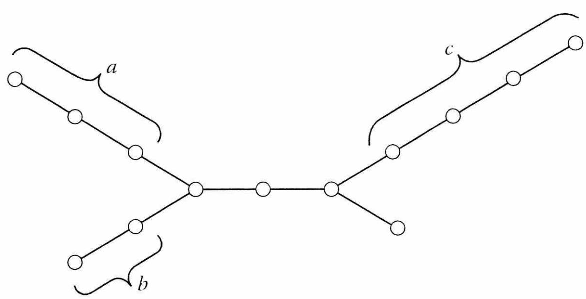

FIGURE 9.5: Graph $H_{a,b,c}$.

Let $\ell \in \{j, k, j+k\}$. Since for every integers j and k the inequality $3j^2+3k^2-3jk+\ell \geq 0$ holds, we see that $a, b, c \geq 128$ in Theorem 9.7.7. Therefore, the smallest graph satisfying the assumptions is $H_{128,128,128}$ on 388 vertices, obtained when $j = k = 0$.

The case $i = 3$ and T being homeomorphic either to the claw or H is rather interesting. In some cases (when there are not *many* long rays), we can prove $W(L^3(T)) > W(T)$, but in other ones, only the congruence arguments yield $W(L^3(T)) \neq W(T)$. These results are summarized in [46] in the following two statements.

Theorem 9.7.8 *Let T be a tree homeomorphic to $K_{1,3}$. Then, $W(L^3(T)) \neq W(T)$.*

Theorem 9.7.9 *Let G be a graph homeomorphic to H. Then, the equation $W(L^3(G)) = W(G)$ has a solution if and only if G is of type $H_{a,b,c}$ as stated in Theorem 9.7.7.*

These statements not only disprove Conjecture 9.7.1 (and give a positive answer to Problem 9.7.1) but completely characterize trees T and integers $i \geq 3$ such that $W(L^i(T)) = W(T)$. This may be surprising since for $i = 2$, we do not know answers to much weaker problems (see the previous section).

We conclude this chapter with two problems.

Problem 9.7.2 *Find all graphs (with cycles) G and powers i for which*

$$W(L^i(G)) = W(G).$$

This problem for $i = 1$ is obviously very rich with many different solutions, so it probably will not be possible to find all of them. But still, stating it as a problem could serve as a motivation for searching of various graph classes that satisfy the equation. Nevertheless, we want to emphasize the case $i \geq 2$. In this case, the problem is still rich with many solutions, particularly among the trees, but abandoning the class of trees can reduce the solutions significantly. At the moment, cycles are the only known cyclic graphs G for which $W(L^i(G)) = W(G)$ holds for some $i \geq 3$. Thus, we formulate another, much weaker problem:

Problem 9.7.3 *Let $i \geq 3$. Is there a graph G, different from a cycle and a tree, such that*

$$W(L^i(G)) = W(G)?$$

9.8 Summary and Conclusion

In this chapter, we studied the Wiener index of graphs and their (iterated) line graphs and also some related problems. Although the situation is completely solved for trees and their iterated line graphs, other than quadratic, for general graphs, the problem is still open. Of course, from the chemist's perspective, important role is played by *chemical graphs* and by graphs that do not have many cycles. We expect that this area can be very prolific, producing many nice results in the future.

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