Abstract

The Wiener index is the sum of distances between all pairs of vertices of a connected graph. In this paper we propose $q$-analogs of the Wiener index, motivated by the theory of hypergeometric series. The basic properties of these $q$-Wiener indices are established, as well as their relations with the Hosoya polynomial. Some possible chemical interpretations and applications of the $q$-Wiener indices are considered.

1 Introduction

In this paper we are concerned with simple graphs, and all graphs considered are assumed to be connected. Let $G$ be such a graph, with $V(G)$ and $E(G)$ being its vertex and edge sets, respectively. The number of vertices of $G$, i.e., $|V(G)|$, is denoted by $n = n(G)$.

The distance between two vertices $u$ and $v$, denoted by $d(v,u)$, is the length of a shortest path between $v$ and $u$. Then the Wiener index of $G$ is

$$W = W(G) = \sum_{(v,u) \subseteq V(G)} d(v,u)$$
which also could be written as

$$W = W(G) = \sum_{k \geq 1} k d(G, k)$$

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

For details of the mathematical theory of the Wiener index and its chemical applications see [1–4]; for some recent works along these lines see [5–10].

The aim to this paper is to study the $q$-analog of the Wiener index. The earliest $q$-analog studied in detail is the basic hypergeometric series, which was introduced in the 19th century [11].

A $q$-analog is, roughly speaking, a theorem or identity in the variable $q$ that gives back a known result in the limit, as $q \to 1$ (from inside the complex unit circle in most situations).

$q$-Analogs find applications in a number of areas, including the study of fractals and multi-fractal measures, and expressions for the entropy of chaotic dynamic systems. $q$-Analogs also appear in the study of quantum groups and in $q$-deformed superalgebras [12,13].

2 Definitions and Basic Properties

2.1 $q$-Wiener index

Let $q$ be a positive real number, $q \neq 1$. We define the $q$-analog of $k$, also known as the $q$-bracket or $q$-number of $k$, to be

$$[k]_q = \frac{1 - q^k}{1 - q} = \sum_{0 \leq i < k} q^i = 1 + q + q^2 + \cdots + q^{k-1}.$$  \hspace{1cm} (2)

Then $\lim_{q \to 1} [k]_q = k$.

Based on this formalism, one can conceive the $q$-analog of the Wiener index as

$$W_1(G, q) = \sum_{\{v, u\} \subseteq V(G)} [d(v, u)]_q.$$

In what follows we shall also consider the second and third $q$-analogs of $W$, defined as

$$W_2(G, q) = \sum_{\{v, u\} \subseteq V(G)} [d(v, u)]_q q^{L - d(v, u)},$$

$$W_3(G, q) = \sum_{\{v, u\} \subseteq V(G)} [d(v, u)]_q q^{d(v, u)}.$$
where \( L \) is the diameter of \( G \). Again, one recovers the usual Wiener index by taking the limit \( q \to 1 \):

\[
\lim_{q \to 1} W_1(G, q) = \lim_{q \to 1} W_2(G, q) = \lim_{q \to 1} W_3(G, q) = W(G) .
\]  

(3)

It is evident that such a generalization of the Wiener–index concept can be further extended by considering

\[
\sum_{\{v,u\} \subseteq V(G)} [d(v,u)]_q \Phi(q, d(v,u))
\]

with \( \Phi(x,y) \) being any function in the variables \( x \) and \( y \), such that \( \lim_{x \to 1} \Phi(x,y) = 1 \) for all values of \( y \). Yet we stop at \( W_1, W_2, \) and \( W_3 \).

Bearing in mind Eqs. (1) and (2), it is straightforward to show that

\[
W_1(G, q) = \sum_{k \geq 1} [k]_q d(G,k) = \sum_{k \geq 1} (1 + q + q^2 + \cdots + q^{k-1}) d(G,k)
\]  

(4)

\[
W_2(G, q) = \sum_{k \geq 1} [k]_q q^{L-k} d(G,k) = \sum_{k \geq 1} (1 + q + q^2 + \cdots + q^{k-1}) q^{L-k} d(G,k)
\]  

(5)

\[
W_3(G, q) = \sum_{k \geq 1} [k]_q q^k d(G,k) = \sum_{k \geq 1} (1 + q + q^2 + \cdots + q^{k-1}) q^k d(G,k)
\]  

(6)

In addition, we have the following relations among the three \( q \)-Wiener indices:

\[
W_1(G, q) = q^{L-1} W_2 \left( G, \frac{1}{q} \right)
\]

\[
W_2(G, q) = q^{L-1} W_1 \left( G, \frac{1}{q} \right)
\]

\[
W_3(G, q) = (1 + q) W_1(q^2) - W_1(G, q)
\]

Let \( v \) and \( u \) be two vertices of the graph \( G \) and let their distance be \( d \). The shortest path between \( v \) and \( u \) can be viewed as a sequence \( d \) mutually incident edges, \( e_1, e_2, \ldots, e_d \), such that \( v \) is an end-vertex of \( e_1 \) and \( u \) and end-vertex of \( e_d \). So, we can go from \( v \) to \( u \) in \( d \) steps, along the edges \( e_1, e_2, \ldots, e_d \). Suppose that the contribution of the first step is unity, of the second step is \( q \), of the third step \( q^2 \), of the \( i \)-th step is \( q^{i-1} \). The contribution obtained by moving along the entire shortest path would then be \( 1+q+q^2+\cdots+q^{d-1} \). This observation may serve for an interpretation of the invariants \( W_1 \), and after an obvious modification, also of \( W_2 \) and \( W_3 \). If the parameter \( q \) is chosen to be positive and less than unity, then the \( q \)-analogs of the Wiener index would provide models for measuring
interactions between individual atoms in a molecule which are known to decrease with their distance.

In connection with the above deliberations, it should be mentioned that in a recent paper [14], a class of invariants of (molecular) graphs was considered, having the form

\[ \tilde{Q} = \sum_{\{v,u\}\subseteq V(G)} f(d(v,u)) \]

where \( f(x) \) depends solely on the distance \( d(u,v) \) between the vertices \( u \) and \( v \). This invariant satisfies the identity

\[ \tilde{Q} = \sum_{k \geq 1} f(k) d(G,k) \]

which should be compared with Eqs. (1) and (4)–(6).

Adopting the standard convention

\[ \sum_{k=m}^{n} a_k = \begin{cases} a_m + a_{m+1} + \cdots + a_n & \text{if } m \leq n \\ 0 & \text{if } m = n + 1 \end{cases} \]

by straightforward calculation we arrive at:

**Proposition 1.** The \( q \)-Wiener indices \( W_1(G,q) \), \( W_2(G,q) \), and \( W_3(G,q) \) are polynomials in \( q \), and

\[ W_1(G,q) = \sum_{k=0}^{L-1} \sum_{j=k+1}^{L} d(G,j) q^k \]

\[ W_2(G,q) = \sum_{k=0}^{L-1} \sum_{j=0}^{k} d(G,L-k+j) q^k \]

\[ W_3(G,q) = \sum_{k=0}^{L-1} \sum_{j=[k/2]+1}^{k} d(G,j) q^k + \sum_{k=L}^{2L-1} \sum_{j=[k/2]+1}^{L} d(G,j) q^k \]

where \( \lfloor \ell \rfloor \) is the greatest integer smaller or equal to \( \ell \).

This proposition shows us that the coefficients of \( q^k \) in \( W_1(G,q) \), \( W_2(G,q) \), and \( W_3(G,q) \) is exactly the numbers of edges of \( G \) that have been weighted with \( q^k \).

In Table 1 are given the coefficients of the polynomial \( W_1(G,q) \) for some alkanes, according to Eq. (7).
Table 1. The coefficients $a_k$ ($0 \leq k \leq 6$), pertaining to $q^k$ in Eq. (7).

<table>
<thead>
<tr>
<th>alkane</th>
<th>$a_0$</th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
<th>$a_4$</th>
<th>$a_5$</th>
<th>$a_6$</th>
<th>$W(G)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-methyloctane</td>
<td>36</td>
<td>28</td>
<td>20</td>
<td>14</td>
<td>9</td>
<td>5</td>
<td>2</td>
<td>114</td>
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<tr>
<td>3-methyloctane</td>
<td>36</td>
<td>28</td>
<td>20</td>
<td>13</td>
<td>8</td>
<td>4</td>
<td>1</td>
<td>110</td>
</tr>
<tr>
<td>4-methyloctane</td>
<td>36</td>
<td>28</td>
<td>20</td>
<td>13</td>
<td>7</td>
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<td>1</td>
<td>108</td>
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<td>45</td>
<td>36</td>
<td>25</td>
<td>18</td>
<td>12</td>
<td>7</td>
<td>3</td>
<td>146</td>
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<tr>
<td>2,3-dimethyloctane</td>
<td>45</td>
<td>36</td>
<td>26</td>
<td>17</td>
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<td>2</td>
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<td>36</td>
<td>26</td>
<td>18</td>
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<tr>
<td>2,2,3-trimethyloctane</td>
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<tr>
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<td>41</td>
<td>26</td>
<td>14</td>
<td>6</td>
<td>2</td>
<td>210</td>
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</tbody>
</table>

From Table 1 we see that 2,2,3-trimethyloctane and 2,2,4-trimethyloctane have equal Wiener indices $W(G)$, but different $W_1(G, q)$. The same is true for 2,3,3-trimethyloctane and 2,3,4-trimethyloctane. This hints toward possible advantages of the $q$-Wiener indices over the ordinary Wiener index.

The vast majority of chemical applications of the Wiener index deal with acyclic organic molecules. Their molecular graphs are trees [15]. In view of this, it is not surprising that in the chemical literature there are numerous studies of properties of the Wiener indices of trees.

A tree is a connected acyclic graph. Each pair of vertices of a tree is connected by a unique path. A vertex of degree one is called a pendent vertex. A tree on $n$ vertices has at least 2 and at most $n - 1$ pendent vertices. The (unique) $n$-vertex trees with 2 and $n - 1$ pendent vertices are the path and the star, respectively, denoted by $P_n$ and $S_n$, respectively. For these trees we have:
Proposition 2. For \( n \geq 2 \),

\[
W_1(S_n, q) = \binom{n}{2} + \binom{n-1}{2} q
\]

\[
W_2(S_n, q) = \binom{n-1}{2} + \binom{n}{2} q
\]

\[
W_3(S_n, q) = (n - 1)q + \binom{n-1}{2} q^2 + \binom{n-1}{2} q^3
\]

\[
W_1(P_n, q) = \binom{n}{2} + \binom{n-1}{2} q + \binom{n-2}{2} q^2 + \cdots + q^{n-2}
\]

\[
W_2(P_n, q) = 1 + \binom{3}{2} q + \binom{4}{2} q^2 + \cdots + \binom{n}{2} q^{n-2}
\]

\[
W_3(P_n, q) = \sum_{k=1}^{n-2} \frac{1}{2} \left( 2n - k - \left\lfloor \frac{k}{2} \right\rfloor - 1 \right) \left( k - \left\lfloor \frac{k}{2} \right\rfloor \right) q^k + \sum_{k=n-1}^{2n-3} \left( n - \left\lfloor \frac{k}{2} \right\rfloor \right) q^k.
\]

### 2.2 q-Multiplicative Wiener index

Few years ago the multiplicative version of the Wiener index, denoted by \( \pi(G) \), was put forward [16]. This molecular structure descriptor is equal to the product of the distances of all pairs of vertices of the underlying molecular graph, i.e.,

\[
\pi(G) = \prod_{\{v,u\} \subseteq V(G)} d(v, u).
\]

Since this index is, even for small molecular graphs, rather large number, e.g. 34,560 for the hexane graph \( (P_6) \), in QSPR/QSAR modeling it is convenient to work with \( \log \pi(G) \) instead of \( \pi(G) \). Of course,

\[
\log \pi(G) = \sum_{\{v,u\} \subseteq V(G)} \log d(v, u) = \sum_{k \geq 1} (\log k) d(G,k).
\]

The \( q \)-anologs of the multiplicative Wiener index are defined in full analogy with \( W_i(G, q) \), \( i = 1, 2, 3 \):

\[
\pi_1(G, q) = \prod_{\{v,u\} \subseteq V(G)} [d(v, u)]_q = \prod_{k \geq 1} \{[k]_q\}^{d(G,k)}
\]

\[
\pi_2(G, q) = \prod_{\{v,u\} \subseteq V(G)} [d(v, u)]_q q^{L-d(v,u)} = \prod_{k \geq 1} \{[k]_q q^{L-k}\}^{d(G,k)}
\]

\[
\pi_3(G, q) = \prod_{\{v,u\} \subseteq V(G)} [d(v, u)]_q q^{d(v,u)} = \prod_{k \geq 1} \{[k]_q q^{k}\}^{d(G,k)}
\]
from which it immediately follows:

\[
\log \pi_1(G, q) = \sum_{k \geq 1} \left( \log \frac{1-q^k}{1-q} \right) d(G, k)
\]

\[
\log \pi_2(G, q) = \sum_{k \geq 1} \left( \log \frac{1-q^k}{1-q} \right) d(G, k) + \binom{n}{2} L \log q - W(G) \log q
\]

\[
\log \pi_3(G, q) = \sum_{k \geq 1} \left( \log \frac{1-q^k}{1-q} \right) d(G, k) + W(G) \log q .
\]

3 Relations between q-Wiener Indices and Hosoya Polynomial

The counting polynomial

\[ H(G, \lambda) = \sum_{k=1}^{L} d(G, k) \lambda^k \]  \hspace{1cm} (8)

was first put forward by Hosoya [17]. Hosoya himself called it “Wiener polynomial”, but eventually the more appropriate name “Hosoya polynomial” has been accepted.

Combining Eq. (8) with the definitions of the \( q \)-Wiener indices, we arrive at:

**Proposition 3.** Let \( G \) be a connected graph on \( n \) vertices. Then

\[
W_1(G, q) = \frac{1}{1-q} \left[ \binom{n}{2} - H(G, q) \right]
\]

\[
W_2(G, q) = \frac{q^L}{1-q} \left[ H \left( G, \frac{1}{q} \right) - \binom{n}{2} \right]
\]

\[
W_3(G, q) = \frac{1}{1-q} \left[ H(G, q) - H(G, q^2) \right].
\]

The most famous property of the Hosoya polynomial is that its first derivative at \( \lambda = 1 \) is equal to the Wiener index [17]. The analogous relations between the derivatives of the \( q \)-Wiener indices and the Hosoya polynomial are stated in:

**Proposition 4.** Let \( G \) be a connected graph. Then,

\[
W'_1(G, q) = \frac{1}{1-q} \left[ W_1(G, q) - H'(G, q) \right]
\]

\[
W'_2(G, q) = \frac{1}{1-q} \left\{ W_2(G, q) + L q^{L-1} \left[ H \left( G, \frac{1}{q} \right) - \binom{n}{2} \right] - q^{L-2} H' \left( G, \frac{1}{q} \right) \right\}
\]

\[
W'_3(G, q) = \frac{1}{1-q} \left[ W_3(G, q) + H'(G, q) - 2q H'(G, q^2) \right].
\]
By taking the limit $q \to 1$, we get:

$$
W'_1(G, 1) = \frac{1}{2} H''(G, 1)
$$

$$
W'_2(G, 1) = \frac{1}{2} \left[ (2L - 2)H'(G, 1) - H''(G, 1) \right]
$$

$$
W'_3(G, 1) = \frac{1}{2} \left[ 2H'(G, 1) + 3H''(G, 1) \right].
$$

Before stating the next properties, we need to define the partial Hosoya polynomial $H_m(G, \lambda)$, defined as

$$
H_m(G, \lambda) \equiv 0 \quad \text{if } m = 0
$$

$$
H_m(G, \lambda) = \sum_{k=1}^{m} d(G, k) \lambda^k \quad \text{if } m = 1, 2, 3, \ldots, L.
$$

We see that $H_L(G, \lambda) = H(G, \lambda)$ and $H_L(G, 1) = \binom{n}{2}$.

**Proposition 5.** Let $G$ be a connected graph. Then,

$$
W_1(G, q) = \sum_{k=0}^{L-1} \left[ H_L(G, 1) - H_k(G, 1) \right] q^k
$$

$$
W_2(G, q) = \sum_{k=0}^{L-1} \left[ H_L(G, 1) - H_{L-k-1}(G, 1) \right] q^k
$$

$$
W_3(G, q) = \sum_{k=0}^{2L-1} \left[ H_L(G, 1) - H_{\lfloor k/2 \rfloor}(G, 1) \right] q^k - \sum_{k=0}^{L-1} \left[ H_L(G, 1) - H_k(G, 1) \right] q^k.
$$

Bearing in mind the limit values (3), we arrive at the following interesting corollary of Proposition 5:

$$
W(G) = \sum_{k=0}^{L-1} \left[ H_L(G, 1) - H_k(G, 1) \right].
$$

**Acknowledgements.** This study was supported in part by the Shandong Natural Science Foundation (ZR2010AM020) and in part by the Serbian Ministry of Science and Education (Grant No. 174033).
References


