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ON q-WIENER INDEX OF UNICYCLIC GRAPHS*†

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Abstract

The q-Wiener index of unicyclic graphs are determined in this work. As an example of its applications, an explicit expression of q-Wiener index of caterpillar cycles is presented.

Keywords q-Wiener index; unicyclic graphs; caterpillar cycles

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1 Introduction

All graphs considered in this paper are connected and simple. As usual, the distance between two vertices u, v of a graph G is denoted by $d_G(u,v)$, or $d(u,v)$ for short. The maximum of such numbers, denoted by $d(G)$, is called the diameter of graph G.

Let $u_0u_1u_2\cdots u_n$ be a molecular chain. Note the interaction between two atoms decreases when the distance between them increases. Let $q<1$ be a positive real number, and suppose that the contribution of atom u_1 to atom u_0 is unity. Then the total interaction of atoms to atom u_0 can be modeled by

$$[n+1]_q = 1+q+q^2+\cdots+q^n = \frac{1-q^{n+1}}{1-q}.$$

And the total interaction between individual atoms of a molecule with graph G can be modeled by the following formula [1,2]

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

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In [1,2], other two concepts of q-Wiener index of a graph G are also introduced as follows

$$W_2(G,q) = \sum_{\{u,v\}\in V(G)} [d(u,v)]_q q^{d-d(u,v)},$$
$$W_3(G,q) = \sum_{\{u,v\}\in V(G)} [d(u,v)]_q q^{d(u,v)}.$$

On the one hand, these three q-Wiener indices have close relationship with the classic Wiener index, which can be exemplified by the following equations

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

On the other hand, these three q-Wiener indices are also mutually related as follows

$$W_2(G,q) = q^{d-1} W_1\Big(G, \frac{1}{q}\Big), \tag{1}$$
$$W_3(G,q) = (1+q)W_1(G,q^2) - W_1(G,q). \tag{2}$$

The earliest q-analog studied in detail is the basic hypergeometric series, which was introduced in the 19th century [3]. q-Analogs find their applications in lots of areas, such as fractals and multi-fractal measures, the entropy of chaotic dynamical systems, and quantum groups. For derails in this field, the readers are suggested to refer to [4,5] for example. Based on equations (1) and (2), in this work, we only consider the first case of q-Wiener index. As a result, the q-Wiener index of unicyclic graphs are determined. As an example of its applications, an explicit expression of q-Wiener index of caterpillar cycles is also presented.

Before proceeding, let us introduce some more symbols and terminology. For any complete graph K_n and a forest F, let K_n^F denote the graph obtained by pasting one vertex of K_n and a vertex of T. For any two trees T_1 and T_2 with $u \in V(T_1)$ and $v \in V(T_2)$, let T_1uvT_2 denote a graph obtained by joining T_1 and T_2 with an new edge uv. In this paper, we shall obtain a q-Wiener index of K_n^F at first, and then use the obtained observation to determine the q-winer index of unicyclic graphs. For other symbols and terminology not specified herein, we follow that of [6].

2 q-Wiener Index of Unicyclic Graphs

For any two vertices of u and v of G, we write $d_G(u,v;q) = [d(u,v)]_q$ and $d_G(u;q) = \sum_{v\in V(G)} d_G(u,v;q)$, then

$$W_1(G,q) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v;q) = \frac{1}{2}\sum_{u\in V(G)} d_G(u;q).$$

When $q = 1$, we have

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} d_G(u; 1).$$

For simplicity, we write $W_1(G)$ for $W_1(G, q)$ in this paper.

Lemma 2.1[1] *Let T_1 and T_2 be two trees on n_1 and n_2 vertices, respectively, with $v_1 \in V(T_1)$ and $v_2 \in V(T_2)$. If the tree T is obtained by linking v_1 and v_2 with an edge, then*

$$\begin{aligned} W_1(T) = {} & W_1(T_1) + W_1(T_2) + n_1 n_2 + q(n_1 d_{T_2}(v_2; q) + n_2 d_{T_1}(v_1; q)) \\ & - q(1-q) d_{T_1}(v_1; q) d_{T_2}(v_2; q). \end{aligned}$$

Lemma 2.2 *If we denote by $\{v_1, v_2, \cdots, v_n\}$ the vertex set of the subgraph K_n of K_n^F, by T_i the component of $K_n^F - E(K_n)$ that contains vertex v_i and $n_i = |T_i|$, then*

$$\begin{aligned} W_1(K_n^F) = {} & \sum_{\substack{i,j=1 \\ i \neq j}}^{n} (n_i n_j + q(n_i d_{T_j}(v_j; q)) + n_j d_{T_i}(v_i; q)) \\ & - \sum_{\substack{i,j=1 \\ i \neq j}}^{n} q(1-q) d_{T_i}(v_i; q) d_{T_j}(v_j; q) + \sum_{i=1}^{n} W_1(T_i). \end{aligned}$$

Proof Let $G = K_n^F$. By (1) of Lemma 2.1, we have

$$\begin{aligned} W_1(K_n^F) = {} & \sum_{\{u,v\} \subseteq V(K_n^F)} d_G(u, v; q) \\ = {} & \sum_{i=1}^{n} \sum_{\{u,v\} \subseteq V(T_i)} d_G(u, v; q) + \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \sum_{\substack{u \in V(T_i) \\ v \in V(T_j)}} d_G(u, v; q) \\ = {} & \sum_{\substack{i \neq j \\ i,j=1}}^{n} \left(\sum_{\substack{u \in V(T_i) \\ v \in V(T_j)}} d_G(u, v; q) + \sum_{\{u,v\} \subseteq V(T_i)} d_G(u, v; q) + \sum_{\{u,v\} \subseteq V(T_j)} d_G(u, v; q) \right) \\ & - \sum_{\substack{i \neq j \\ i,j=1}}^{n} \left(\sum_{\{u,v\} \subseteq V(T_i)} d_G(u, v; q) + \sum_{\{u,v\} \subseteq V(T_j)} d_G(u, v; q) \right) + \sum_{i=1}^{n} W_1(T_i) \end{aligned}$$

$$= \sum_{i=1}^{n} W_1(T_i) + \sum_{\substack{i,j=1 \\ i \neq j}}^{n} W_1(T_i v_i v_j T_j) - (n-1) \sum_{i=1}^{n} W_1(T_i)$$

$$= \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \big(W_1(T_i) + W_1(T_j) + n_i n_j + q(n_i d_{T_j}(v_j;q) + n_j d_{T_i}(v_i;q))$$

$$-q(1-q) d_{T_i}(v_i;q) d_{T_j}(v_j;q)\big) - (n-2) \sum_{i=1}^{n} W_1(T_i)$$

$$= \sum_{\substack{i,j=1 \\ i \neq j}}^{n} (n_i n_j + q(n_i d_{T_j}(v_j;q) + n_j d_{T_i}(v_i;q)))$$

$$- \sum_{\substack{i,j=1 \\ i \neq j}}^{n} (q(1-q) d_{T_i}(v_i;q) d_{T_j}(v_j;q)) + \sum_{i=1}^{n} W_1(T_i).$$

And so, the lemma follows.

Theorem 2.1 *Let G be a unicyclic graph with cycle $C = v_1 v_2 \cdots v_n v_1$. If T_i is the subgraph of $G - E(C)$ that contains vertex v_i and $n_i = |T_i|$, then*

$$W_1(G) = \sum_{\substack{i,j=1 \\ i \neq j}}^{n} (n_i n_j + q(n_i d_{T_j}(v_j;q) + n_j d_{T_i}(v_i;q)))$$

$$- \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \big(q(1-q) d_{T_i}(v_i;q) d_{T_j}(v_j;q) q^{d_C(v_i,v_j)-1}$$

$$+ n_i n_j [d_C(v_i, v_j) - 1]_q\big) + \sum_{i=1}^{n} W_1(T_i).$$

Proof Add as few as possible edges to G such that in the new obtained graph G', every vertex v_i is adjacent to every vertex v_j with $i \neq j$. For every pair of vertices $u \in V(T_i)$ and $v \in V(T_j)$, we have

$$d_G(u,v) = d_{G'}(u,v) + d_C(v_i,v_j) - 1.$$

Combining this observation with the definition of $d_G(u,v;q)$, we have

$$d_G(u,v;q) = d_{G'}(u,v;q) q^{d_C(v_i,v_j)-1} + [d_C(v_i,v_j) - 1]_q.$$

And so,

$$\begin{aligned}W_1(G) &= \sum_{\substack{i,j=1\\ i\neq j}}^{n} \sum_{\substack{u\in V(T_i)\\ v\in V(T_j)}} d_G(u,v;q) + \sum_{i=1}^{n} \sum_{\{u,v\}\subseteq V(T_i)} d_G(u,v;q)\\ &= \sum_{\substack{i,j=1\\ i\neq j}}^{n} \big((W_1(T_iv_iv_jT_j) - W_1(T_i) - W_1(T_j))q^{d_C(v_i,v_j)-1}\\ &\qquad +n_in_j[d_C(v_i,v_j)-1]_q\big) + \sum_{i=1}^{n} W_1(T_i).\end{aligned}$$

It follows from the combination of Lemma 2.1 and the above formula that

$$\begin{aligned}W_1(G) = \sum_{i=1}^{n} W_1(T_i) + &\sum_{\substack{i,j=1\\ i\neq j}}^{n} \big((n_in_j + q(n_id_{T_j}(v_j;q) + n_jd_{T_i}(v_i;q))\\ &-q(1-q)d_{T_i}(v_i;q)d_{T_j}(v_j;q))q^{d_C(v_i,v_j)-1} + n_in_j[d_C(v_i,v_j)-1]_q\big).\end{aligned}$$

And so, the theorem follows.

As an application of Theorem 2.1, we shall present the explicity expression of the caterpillar cycles. This kind of graphs are constructed as follows [5]. Let $C_k = v_1v_2\cdots v_kv_1$ be a cycle on k vertices with $k \geq 3$. Then caterpillar cycle $C_k(n_1, n_2\cdots n_k)$ is obtained from C_k by attaching n_i vertices to v_i, where $n_i \geq 0$ for all $i = 1, 2, \cdots, k$.

Lemma 2.3[1,2] *If $n \geq 2$, then*

$$W_1(S_n) = \frac{n(n-1)}{2} + \frac{(n-1)(n-2)}{2}q.$$

The following corollary follows directly from the combination of Theorem 2.1 and Lemma 2.3, and so we leave its proof to the readers.

Corollary 2.1 *Let $C_k(n_1, n_2, \cdots, n_k)$ be a caterpillar cycle with $k \geq 3$, $n_i \geq 0$ for all $i = 1, 2, \cdots, k$. If denote by $C = v_1v_2\cdots v_kv_1$ the unique cycle of this caterpiller cycle, and T_i by the tree of $C_k(n_1, n_2, \cdots, n_k) - E(C)$ that contains vertex v_i, then*

$$\begin{aligned}W_1(G) = &\frac{1}{2}\sum_{i=1}^{n} \big(n_i(n_i-1) + (n_i-1)(n_i-2)q\big)\\ &+ \sum_{\substack{i,j=1\\ i\neq j}}^{n} \big((n_in_j + q(2n_in_j - n_i - n_j) - q(1-q)(n_i-1)(n_j-1))q^{d_C(v_i,v_j)-1}\\ &+n_in_j[d_C(v_i,v_j)-1]_q\big).\end{aligned}$$

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