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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

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