Wiener Index of Sodium Chloride and Benzenoid Structures

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Abstract

The topological descriptor Wiener index named after the chemist Harold Wiener is defined as half the sum of the distances between every pair of vertices of a graph. A lot of research has been devoted to finding Wiener index by brute force method. In this paper we compute the wiener index of chemical structures such as sodium chloride and benzenoid without using distance matrix.

Keywords: Wiener index, embedding, sodium chloride, honeycomb.

1 Introduction

Graph representation of molecular structures is widely used in computational chemistry. Trinajstic noted that the roots of chemical graph theory may be found in the works by chemists of 18-19th centuries such as Higgins, Kopp, Crum Brown. First chemical graphs for representing molecules were used by them.

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. The vertices in G are connected by an edge if there exists an edge $uv \in E(G)$ connecting the vertices u and v in G such that $u, v \in V(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The number of vertices and edges in a graph will be denoted by $|V(G)|$ and $|E(G)|$, respectively.

To identify molecular structures of chemical compound, the molecular graph invariants, called topological indices could be used too. Topological indices are designed basically by transforming a molecular graph into a

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number. The first use of a topological index was made in 1947 by the chemist Harold Wiener. Wiener introduced the notion of path number of a graph as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. Wiener originally defined his index (W) on trees and studied its use for correlations of physico-chemical properties of alkanes, alcohols, amines and their analogous compounds.

Hosoya reformulated the wiener index in terms of distance between vertices in an arbitrary graph. He defined W as the sum of distances between all pairs of vertices of the graph under consideration, $W(G) = \sum_{u,v} d(u,v)$, where $d(u,v)$ is the number of edges in a minimum path connecting the vertices u and v.

In the initial applications, the Wiener Index is employed to predict physical parameters such as boiling points, heats of information, heats of vaporization, molar volumes and molar refractions of alkanes [5, 21]. The study of Wiener index is one of the current areas of research in mathematical chemistry (see, for example [2]). Researchers made some attempts to device a technique to find Wiener index of chemical compounds [2, 5, 9, 10, 11, 13, 21]. They also used brute force method based on distance matrix to compute the same [25].

In theoretical computer science, Weiner index is considered as one of the basic descriptors of fixed interconnection networks because it provides the average distance between any two nodes of the network. So far, most of the researchers apply brute force method to compute Weiner index [8, 9, 10, 23]. Some researchers devised techniques to find Weiner index of certain fixed interconnection networks [8, 15, 23]. Isometric embeddings of benezoid graphs are surveyed in [18]. Their embeddings into hypercubes provide methods for computing the Wiener index of partial cubes [18]. However, these techniques cannot be applied to other networks. To our knowledge, there is no unified technique to compute Wiener Index of graphs. This motivated Bojan Mohar and Toniaz Pisanski to throw an open problem "is there an algorithm for general graphs that would calculate the Wiener index without calculating the distance matrix?". This open problem was posed in 1988 in Journal of Mathematical Chemistry [6]. It remains unsolved until now. Our objective of this paper is to find a mathematical technique to compute the Wiener index without using the distance matrix, which also generalizes the existing techniques.

2 The Partition Lemma

The *Wiener index* $WI(G)$ of a graph G is defined by

$$WI(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u,v),$$

where the summation extends over all possible pairs of distinct vertices u and v of G.

We apply a partition strategy and use embedding as a tool to establish an elegant technique to compute Wiener index of certain classes of graphs. We begin with certain definitions of embedding parameters.

An *embedding* [3] of a guest graph $G(V,E)$ into a host graph $H(V,E)$ is defined by an injective function $f : V(G) \to V(H)$ together with a mapping P_f which assigns to each edge (u,v) of G a path $P_f(f(u), f(v))$ between $f(u)$ and $f(v)$ in H.

The *dilation-sum* $\widetilde{D_f}(G,H)$ of an embedding f of G into H is defined as

$$\widetilde{D_f}(G,H) = \sum_{u,v \in E(G)} d_H(f(u), f(v)),$$

where $d_H(f(u), f(v))$ is the length of the path $P_f(f(u), f(v))$ in H.

Then the *minimum dilation-sum* of G into H is defined as

$$\widetilde{D}(G,H) = \min_f \widetilde{D_f}(G,H),$$

where the minimum is taken over all embeddings f of G into H.

The *congestion* of an embedding f of G into H is the maximum number of edges of the guest graph that are embedded on any single edge of the host graph. Let $C_f(G,H(e))$ denote the number of edges (u,v) of G such that e is in the path $P_f(f(u), f(v))$. In other words,

$$C_f(G,H(e)) = |\{(u,v) \in E(G) : e \in P_f(f(u), f(v))\}|.$$

For $S \subseteq E(H)$, the congestion on S is the sum of the congestions on the edges in S.

The *congestion-sum* $\widetilde{C_f}(G,H)$ of an embedding f of G into H is defined as

$$\sum_{e \in E(H)} C_f(G,H(e)).$$

Then the *minimum congestion-sum* of G into H is defined as

$$\widetilde{C}(G,H) = \min_f \widetilde{C_f}(G,H),$$

where the minimum is taken over all embeddings f of G into H.

For any embedding, the congestion-sum and the dilation-sum are one and the same [17]. This motivated the following lemma.

Lemma 1 (Partition Lemma) *[16]Let G be a graph of order n. Let $\{S_1, S_2, ..., S_p\}$ be a partition of $E(G)$ such that each S_i is an edge cut of G and the removal of edges of S_i leaves G into 2 components G_i and G_i'. Also each S_i satisfies the following conditions:*

(i) For any two vertices $u, v \in G_i$, a shortest path between u and v has no edges in S_i.

(ii) For any two vertices $u, v \in G_i'$, a shortest path between u and v has no edges in S_i.

(iii) For any two vertices $u \in G_i$ and $v \in G_i'$, a shortest path between u and v has exactly one edge in S_i.

Then $WI(G) = \sum_{i=1}^{p} |V(G_i)|\,(n - |V(G_i)|)$. ■

3 Computing Wiener Index

In this section we describe an efficient method of computing Wiener Index of chemical structures such as sodium chloride, honeycomb and benzenoid graphs.

3.1 Sodium Chloride (Nacl)

In our day-to-day life, the common salt $Nacl$ is used as an important preservative because it retards the growth of microorganiasm. It also improves the flavour of food items. Chlorine products are used in metal cleaners, paper bleach, plastics and water treatment. They are also used in medicines. A three dimensional mesh $M(m,n,k)$ is defined as the cartesian product $P_m \times P_n \times P_k$. In a three dimensional mesh there are mnk number of vertices and $(2mn - m - n)k + (k-1)mn$ number of edges. We find that the unit cell representation of Sodium chloride ($Nacl$) is the same as the three dimensional mesh $M(3,3,3)$. Infact in Figure 1 the hollow circles represent Na^+ and solid circles represent Cl^- ions.

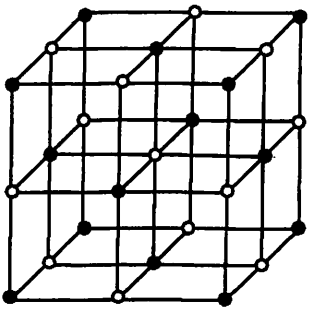

Figure 1: Three dimensional mesh $M(3,3,3)$

Let the vertex set of $M(m,n,k)$ be the set $V = \{x_1x_2x_3 : 0 \leq x_1 \leq m-1, 0 \leq x_2 \leq n-1, 0 \leq x_3 \leq k-1\}$ and two vertices $x = x_1x_2x_3$ and $y = y_1y_2y_3$ are linked by an edge if $\sum_{i=1}^{3} |x_i - y_i| = 1$.

Theorem 1 $WI(M(m,n,k)) = \frac{mnk}{6}[nk(m^2-1)+mk(n^2-1)+mn(k^2-1)]$.

Proof. For $1 \leq i \leq m-1$, let A_i be an edge cut of $M(m,n,k)$ such that A_i disconnects $M(m,n,k)$ into two components X_i and X_i' where $V(X_i) = \{x_1x_2x_3 : 0 \leq x_1 \leq i-1, 0 \leq x_2 \leq n-1, 0 \leq x_3 \leq k-1\}$. For $1 \leq i \leq n-1$, let B_i be an edge cut of $M(m,n,k)$ such that B_i disconnects $M(m,n,k)$ into two components Y_i and Y_i' where $V(Y_i) = \{x_1x_2x_3 : 0 \leq x_1 \leq m-1, 0 \leq x_2 \leq i-1, 0 \leq x_3 \leq k-1\}$. For $1 \leq i \leq k-1$, let C_i be an edge cut of $M(m,n,k)$ such that C_i disconnects $M(m,n,k)$ into two components Z_i and Z_i' where $V(Z_i) = \{x_1x_2x_3 : 0 \leq x_1 \leq m-1, 0 \leq x_2 \leq n-1, 0 \leq x_3 \leq i-1\}$. The edge cuts A_i, B_i, C_i satisfy the conditions of the Partition Lemma. Thus $WI(M(m,n,k)) = \sum_{i=1}^{m-1} mni(mnk - mni) + \sum_{i=1}^{n-1} mki(mnk - mki) + \sum_{i=1}^{k-1} nki(mnk - nki) = \frac{mnk}{6}[nk(m^2-1)+mk(n^2-1)+mn(k^2-1)]$.

■

3.2 A Benzenoid Structure

Honeycomb mesh can be thought of as a benzenoid structure and can be built from hexagons in various ways. The simplest way to define them

is to consider the portion of the hexagonal tessellation, which is inside a given convex polygon. To maximize symmetry, honeycomb (hexagonal) meshes can be built as follows: One hexagon is a honeycomb mesh of size one, denoted HM_1. See Figure 2(a). The edges of HM_1 are in 3 different directions. If the perpendicular bisectors of these edges meet at point O, then O is called the centre of the honeycomb mesh HM_1. The honeycomb mesh HM_2 of dimension two is obtained by adding six hexagons to the boundary edges of HM_1. See Figure 2(b). Inductively, honeycomb mesh HM_d of dimension d is obtained from HM_{d-1} by adding a layer of hexagons around the boundary of HM_{d-1}. Alternatively, the dimension d of HM_d is determined as the number of hexagons between the center and boundary of HM_d (both inclusive). The number of vertices and edges of HM_d are $6d^2$ and $9d^2 - 3d$ respectively [19]. Further O is considered to be the centre of HM_d, for any d.

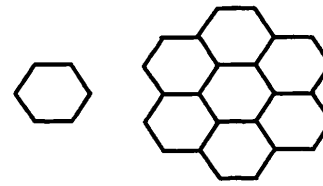

Figure 2: Honeycomb Mesh

Theorem 2 *Let G be the honeycomb mesh HM_d of dimension d. Then*

$$WI(G) = 6\left[\sum_{i=1}^{d-1}\mu_i(6d^2 - \mu_i)\right] + 3\mu_0^2,$$

where $\mu_i = (d-i)(3d-i), 0 \leq i \leq d-1$.

Proof. For convenience we shall introduce a coordinate system for the honeycomb mesh. Let O be the centre of HM_d. Through O draw 3 lines perpendicular to the 3 edge directions and name them as α, β and γ lines. See Figure 3. The α line through O, denoted by α_0, passes through $2d-1$ hexagons. Any line parallel to α_0 and passing through $2d-1-i$ hexagons is denoted by α_i, $1 \leq i \leq d-1$ if the hexagons are in the clockwise sense about α_0 and by α_{-i}, $1 \leq i \leq d-1$ if the hexagons are in the anti-clockwise

sense about α_0. In the same way β_j and β_{-j}, $0 \leq j \leq d-1$, and γ_k and γ_{-k}, $0 \leq k \leq d-1$, are defined.

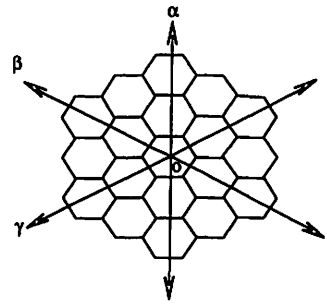

Figure 3: Axes of 3 - Dimensional Honeycomb HM_3

Let E_γ denote the set of edges of HM_d cut by line γ. Then $\{E_{\alpha_0}, E_{\alpha_1}, ..., E_{\alpha_{d-1}}, E_{-\alpha_1}, ..., E_{-\alpha_{d-1}}, E_{\beta_0}, E_{\beta_1}, ..., E_{\beta_{d-1}}, E_{-\beta_1}, ..., E_{-\beta_{d-1}}, E_{\gamma_0}, E_{\gamma_1}, ..., E_{\gamma_{d-1}}, E_{-\gamma_1}, ..., E_{-\gamma_{d-1}}\}$ is a partition of the edge set of HM_d and each of its members satisfies the conditions of the Partition Lemma. By the symmetry of HM_d, it is enough to apply the Partition Lemma to the edge cuts $E_{\alpha_0}, E_{\alpha_1}, ..., E_{\alpha_{d-1}}$ to compute the Wiener Index of HM_d. The sum of congestions on $E_{\alpha_0}, E_{\alpha_1}, ..., E_{\alpha_{d-1}}$, is given by $\mu_0^2 + \mu_1(6d^2 - \mu_1) + \mu_2(6d^2 - \mu_2) + ... + \mu_{d-1}(6d^2 - \mu_{d-1})$, where $\mu_i = (d-i)(3d-i), 0 \leq i \leq d-1$. Hence

$$WI(G) = 6\left[\sum_{i=1}^{d-1} \mu_i(6d^2 - \mu_i)\right] + 3\mu_0^2,$$

where $\mu_i = (d-i)(3d-i), 0 \leq i \leq d-1$. ■

4 Conclusion

In this paper an elegant technique has been evolved to compute the wiener index of chemical structures such as sodium chloride and honeycomb without using distance matrix.

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