DOI: 10.2478/auom-2018-0011
An. Şt. Univ. Ovidius Constanţa

VERSITA
Vol. 26(1),2018, 169–187

Exact Formula for Computing the Hyper-Wiener Index on Rows of Unit Cells of the Face-Centred Cubic Lattice

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Abstract

Similarly to Wiener index, hyper-Wiener index of a connected graph is a widely applied topological index measuring the compactness of the structure described by the given graph. Hyper-Wiener index is the sum of the distances plus the squares of distances between all unordered pairs of vertices of a graph. These indices are used for predicting physicochemical properties of organic compounds. In this paper, the graphs of lines of unit cells of the face-centred cubic lattice are investigated. The graphs of face-centred cubic lattice contain cube points and face centres. Using mathematical induction, closed formulae are obtained to calculate the sum of distances between pairs of cube points, between face centres and between cube points and face centres. The sum of these formulae gives the hyper-Wiener index of graphs representing face-centred cubic grid with unit cells connected in a row. In connection to integer sequences, a recurrence relation is presented based on binomial coefficients.

1 Introduction

In mathematical chemistry, Wiener, hyper-Wiener and other topological indices have been introduced. By their help some physical properties, e.g., boil-

Key Words: Hyper-Wiener Index, Face-Centred Cubic Lattice, Shortest Paths, Non-Traditional Grids, Compactness Measures, Topological Graph Indices, Crystal Structure, Sum of Distances, Recurrence relations, Integer sequences.

2010 Mathematics Subject Classification: Primary 05C12, 11Y55; Secondary 05C30, 92E10, 94C15, 82B20.

Received: May, 2017.

Revised: July, 2017.

Accepted: July, 2017.

ing point, can be predicted based on the structure of the molecules. Mathematical and computational methods are successfully used to model and predict the structure of matter in atomic level [5]. The structures of molecules, from mathematical point of view, are graphs. Graph theory is used in almost every field of science and it is also heavily used in practice, both for simulations and engineering solutions. A graph in this context is made up of vertices or nodes and lines called edges that connect them. Digital geometry deals with regular tessellations, i.e., graphs with regular, periodic structures, and in this way, it is closely related to crystallography. Digital geometry has also applications in image processing and computer graphics [12]. The square and cubic grids are assumed to be the traditional grids; theory on them is well developed and they are frequently used in various applications. One of the main directions of research of digital geometry deals with descriptions, coordinate systems, computing distances, relations and applications of non-traditional grids [16][20][21] [22]. Non-traditional 3D grids, for instance, body-centred cubic (bcc), face-centred cubic (fcc) lattices and diamond cubic grid, and their appropriate descriptions play importance in physics, crystallography and chemistry, as well.

1.1 Topological Graph Indices

It is an interesting and important task to connect the molecular structures [17] of various matters to their physical properties. Wiener Index (W) is a graph invariant that belongs to the molecular structure descriptors, called topological indices. Initially, Wiener applied it to predict physical parameters such as boiling points of the paraffins [23]. It is, generally, defined as the sum of the shortest distances between every pair of vertices of a given graph G. Another index, the so-called Hyper-Wiener index, H was also introduced [18] for acyclic graphs. Then, Klein, Lukovits and Gutman [11], generalized Randic's definition for all connected graphs, as a generalization of the Wiener index. For molecules, in general, these indices measure how compact a molecule is for its given weight. The molecule is more compact if its index is less, while the Wiener index is computed as a linear function of the distances, the hyper-Wiener index uses also the second moment of the distances. These indices are widely used by chemists to design molecules with desired properties. Various measurable physical quantities, e.g., heats of vaporization, molar volumes and molar refractions can be characterized by them. There are plenty of researches on Wiener indices, especially, about benzenoid hydrocarbons, graphs with hexagonal structure [9][8]. All the three regular tessellations of the plane were studied in [14]. Recently, the task to compute Wiener indices of various 3D structures is also of high importance [1][2]. Hyper-Wiener index is also frequently used for various graphs.

In this paper, we consider special graphs that are built up from fcc unit cells in a row. The Wiener index together with hyper-Wiener index of these graph are computed. In our graphs the vertices are representing the atoms (or ions), and the edges connect the closest atoms (or ions), they could represent covalent, ionic, etc. bonds, depending on the modelled material.

2 Basic Notions and Definitions

In this paper, all graphs are finite, simple, undirected and connected without loops or multiple edges. For a graph G, we denote by $V(G)$ and $E(G)$ its sets of vertices and edges, respectively. The length of a path P, denoted by $|P|$, is the number of its edges [3]. Let $G = (V, E)$ be a simple connected graph. The distance $d_G(u, v)$ between two vertices u and v is defined as the number of edges on a shortest path connecting u and v. Note that, in a graph, there can be several shortest paths between two vertices. A molecular graph is a set of vertices representing the atoms in a molecule and a set of edges representing the covalent bonds between the atoms. Not only molecules can be represented by graphs: there are some elements that form lattice structures in their crystals. Carbon (in diamond) and Silicon have cubic lattice structure known as the diamond structure, even mathematically their structure is not a lattice. In a similar manner, other crystals can also be modelled by graphs underlining their structure, see, e.g., [1]. The most usual arrangements of the atoms (ions) for metals are the bcc and fcc lattices.

In [23] Wiener introduced the notion of, as he called, path number of a graph. Actually, it was the sum of distances between any two carbon atoms in the molecules in terms of carbon-carbon covalent bonds. Subsequently, the index named after Wiener, is generalised to any graph G as

$$W(G) = \frac{1}{2} \sum d_G(u, v) \tag{1}$$

The sum of shortest distances for each pair of vertices of the graph G: the sum runs over all ordered pairs of vertices, and $d_G(u, v)$ denote the length of a shortest path in G between vertices u and v.

2.1 The Hyper-Wiener Index

In [18] hyper-Wiener index (H) for trees was proposed. In a tree graph there is a uniquely determined path between any two distinct vertices. Let two vertices v and u be given, then the shortest path from u to any vertex may or may not contain v. Similarly, the shortest path from v to any vertex may or may not contain u. Based on this, a tree graph can be partitioned to three parts based on any two distinct vertices: a part "between" the two vertices (including exactly those vertices to which the shortest paths from u and v do not contain the other vertex of them) and two subtrees including u and v, respectively. The original definition of hyper-Wiener index is a sum (for every pair of vertices u and v) of products of the number of vertices belonging to subtrees u and v, respectively. This definition works only for acyclic graphs, the concept was extended to all connected graphs by Klein, Lukovits and Gutman in [11], and they have presented an alternative definition related also to Wiener index. H is also used as a structure-descriptor for predicting physicochemical properties of organic compounds. It is one of the recently conceived distance-based graph invariants, often used for pharmacology, agriculture, environment-protection, etc. [10][4][24]. Its formula suggests that H clearly encodes the "compactness" and the "expansiveness" of the structure given by a graph G. The squared term gives relatively more weight to expanded structures than Wiener index, and therefore, H is a good predictor of effects that depend more than linearly on the physical size of a molecule. The Hyper-Wiener index of G is defined as:

$$H(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum d_G^2(u,v), \qquad (2)$$

where $W(G)$ is the Wiener index of the graph G. Actually, the hyper-Wiener index is the average of the Wiener index and the (unnormalized) second moment distance.

2.2 Face-Centred Cubic (fcc) Lattice

Face-centred cubic (fcc) lattice consists of unit cells that are cubes with an atom at each corner of the cube and an atom in the centre of each face of the cube (see Figure 1, as well). In our graphs vertices (points) represent the atoms; the terms, cube vertices (cube points) and face centres (or face centre points) will be used, respectively. Edges connect the closest (neighbour) atoms. In fact, fcc structure has the largest packing density in the three dimensional space: this is one of the most efficient structures to pack same size spheres in a volume [13][6], as it can be seen in Figure 1 (right). Therefore, this structure is also known as cubic closest-packed crystal structure. Metals with fcc structure include: Aluminium, Copper, Gold, Nickel and Silver.

In this paper, we are using graphs that represent rows of unit cells of the fcc lattice (i.e., the dimension of our space is $n \times 1 \times 1$ unit cells). We recall the following straightforward result from [15], where Wiener-index of the graphs of fcc unit cells is computed.

Proposition 1. *Let n be the number of fcc unit cells connected in a row, the number of all vertices $|v|_{all}$ (cube vertices and face centres) in this graph is*

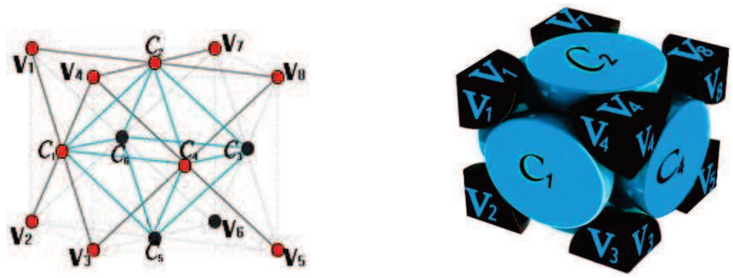

Figure 1: A unit cell (the cube is drawn by broken lines) of face-centred cubic (fcc) lattice (red atoms are on the visible sides of the cube, grey atoms are not on the visible sides) showing the neighbour relation of the atoms (solid lines: grey colour on the faces of the cube and cyan colour inside the cube) (left), and fcc close-packing with spheres (right).

given by $|v|_{all} = (9n+5)$*; the number of cube points is* $|V_b| = (4n+4)$ *and the number of face centers is* $|V_c| = (5n+1)$*.*

The main result of [15], the formula for Wiener index of fcc graphs, is computed as follows.

Proposition 2. *Let n be the number of fcc unit cells that are connected in a row. Then the formula to find W for this graph is:*

$$W(n) = 27n^3 + 45n^2 + 62n + 16. \tag{3}$$

Based on this result, the sequence $W(n)$ can also be found in [19] under code A273322. One can easily check that it is also obtained as a linear recurrence with constant coefficients using the formula

$$W(n) = 4W(n-1) - 6W(n-2) + 4W(n-3) - W(n-4) \text{ for } n > 4$$

based on its first 4 elements.

3 Computing the Hyper-Wiener Index

Based on equations (1) and (2) a small transformation is made on the formula computing H:

$$H(G) = \frac{1}{4} \sum_{u,v \in (G)} (d_G(u,v) + d_G^2(u,v)) \tag{4}$$

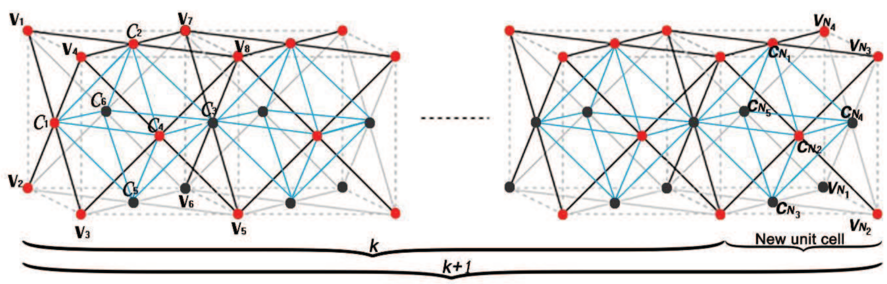

Figure 2: A lying square column of k fcc unit cells connected in a row with a new, $(k+1)$st unit cell attached to the row.

where $d_G(u, v)$ is the distance between the two vertices in the graph. In (4) the distance and the second moment distance are summed. In the following subsections various subsums are computed. Actually, to compute H, the value $d_G(u, v) + d_G^2(u, v)$ is needed for each unordered pair of vertices u and v. For simplifying our notions, we refer for sums of values $d_G(u, v) + d_G^2(u, v)$ as sums of combined distances. In fcc graphs there are two types of vertices. Thus, H is computed based on the sum of the following three subsums of combined distances between

- unordered pairs of face centres,
- pairs of face centres and cube vertices, and
- unordered pairs of cube vertices.

Our proofs use mathematical induction: We compute the subsums for a unit cell, and provide formula for graph containing exactly k unit cells in a row. Then it will be shown that the same formula works for a graph containing $k+1$ unit cells in a row. In proofs we refer to Figure 2. To make our computation more readable and more easily understandable we differentiate two subtypes of face centres:

- the side centres (or side centre points) are located on the side (i.e., on the bottom, top, in front or at back side, i.e., on one of the rectangular side of the square column build by unit cells), e.g., C_2 and C_5 in Figure 2; and
- the shared centres (or shared centre points) are the face centres on the squares, either on the two ends or somewhere inside the body, e.g., C_1 and C_3 in Figure 2.

3.1 Sum of combined Distances between Pairs of Face Centres

Let us start by computing how much the sum of combined distances among face centres increases when a new unit cell is attached to the end of the row (Figure 2).

Lemma 3. *Let k fcc unit cells be connected in a row, and now, a new unit cell is connected to the end of the row to form a graph that represents $k+1$ unit cells in a row. Then the sum of combined distances between pairs of new face centres and between pairs of a new and an old face centres is*

$$\frac{100k^3 + 285k^2 + 251k + 126}{3}. \tag{5}$$

Proof. In our proof, we will calculate the sum of combined distance as follows:

- First of all, and according to Figure 2, the sum of distances between the pairs built up from the new five centre points equals to

$$\frac{1}{2}\sum_{i=1}^{5}\sum_{j=1}^{5} d_G(C_{N_i}, C_{N_j}) = 4\cdot 1 + 4\cdot 1 + 2\cdot 2 = 12$$

  (the distance of the new shared centre C_{N_4} is 1 from the new side centres, e.g. C_{N_1}; there are 4 pairs of neighbour side centres, e.g., C_{N_1} and C_{N_2}; and finally, there are 2 pairs of non-neighbour side centres, e.g., C_{N_1} and C_{N_3}, such that their distances are 2). Consequently, the squares of the distances between the pairs built up from the new five side centre points equals to 16. This is summed up as 12 + 16 = 28.

- Next, we will calculate the distance between the new shared centre (C_{N_4}) and old shared centres (including, e.g., C_1). These distances are the even numbers, and thus, their sum is

  $2\cdot 1 + 4\cdot 1 + 6\cdot 1 + \cdots + 2(k+1)\cdot 1 = 2(1+2+3+\cdots+(k+1)) = \frac{2(k+1)(k+2)}{2} = k^2 + 3k + 2.$

  The sum of their squares is given by

  $2^2\cdot 1 + 4^2\cdot 1 + 6^2\cdot 1 + \cdots + (2(k+1))^2\cdot 1 = 4(1^2+2^2+3^2+\cdots+(k+1)^2) = \frac{4(k+1)(k+2)(2k+3)}{6} = \frac{4k^3+18k^2+26k+12}{3}.$

  The sum of two previous equations:

$$\frac{4k^3 + 18k^2 + 26k + 12}{3} + k^2 + 3k + 2 = \frac{4k^3 + 21k^2 + 35k + 18}{3}.$$

- Next, we will calculate the distance between new side centres and old shared centres. So we have $1+3+5+\cdots+(2k+1)=(k+1)^2$. Then we multiply by 4 since we have 4 new side centres to get the formula $4(k+1)^2$.
  $4(1^2+3^2+5^2+\cdots+(2k+1)^2)=\frac{4(k+1)(2k+1)(2k+3)}{3}=\frac{16k^3+48k^2+44k+12}{3}$.
  The sum of two previous equations:
  $$\frac{16k^3+48k^2+44k+12}{3}+4(k+1)^2=\frac{16k^3+60k^2+68k+24}{3}.$$
- Next, we need to calculate the distance between new side centres (i.e., C_{N_1}, C_{N_2}, C_{N_3} and C_{N_5}) and old side centres. For any of the new side centres we have
  $$2\cdot 4+4\cdot 4+\cdots+(2k\cdot 4)=8+16+24+32+\cdots+8k=$$
  $$8\cdot(1+2+3+\cdots+k)=\frac{8(k(k+1))}{2}=4k^2+4k.$$
  Then we multiply it by 4 since we have 4 new side centres to get the formula $16k^2+16k$. The sum of the squares of these distances can be computed as
  $$4(2)^2+4(4)^2+\cdots+4(2k)^2=4(4+16+36+\cdots+4k^2).$$
  Then we multiply this value also by 4, and we get the formula
  $$\frac{64k^3+96k^2+32k}{3}.$$
  The sum of two previous formulae:
  $$\frac{64k^3+96k^2+32k}{3}+16k^2+16k=\frac{64k^3+144k^2+80k}{3}.$$
- Finally, we will calculate the sum of the distances between the new shared centre, i.e., (C_{N_4}) and all old side centres:
  $4(3+5+7+\cdots+(2k+1))=4((k+1)^2-1)$, and that is, $4k^2+8k$.
  The sum of their squares:
  $$4(3^2+5^2+7^2+\cdots+(2k+1)^2)=\frac{16k^3+48k^2+44k}{3}.$$
  The sum of two previously computed values:
  $$\frac{16k^3+48k^2+44k}{3}+4k^2+8k=\frac{16k^3+60k^2+68k}{3}.$$

The final formula to calculate the sum of total distance between new central points and between new central points and old central points, when we add a new fcc unit cell to the k fcc unit cells connected in a row, is given by:
$28 + \frac{4k^3+21k^2+35k+18}{3} + \frac{16k^3+60k^2+68k+24}{3} + \frac{64k^3+144k^2+80k}{3} + \frac{16k^3+60k^2+68k}{3} =$

$$\frac{100k^3+285k^2+251k+126}{3}.$$

Thus the proof of lemma is finished. □

Lemma 4. *Let n fcc unit cells be connected in a row. Then the sum of combined distances between centre vertices in this fcc grid graph is*

$$\frac{25n^4+45n^3+8n^2+48n}{3}. \tag{6}$$

Proof. The proof goes by induction on the number of unit cells. The base of the induction is the case $n = 1$. In this case, there is only 6 face centres (both side and shared centre points are counted), and the sum of combined distances between these central points equals to 42 (there are 12 pairs of neighbour centres and 3 pairs such that they are opposite to each other, and thus, their distance is 2), and the formula (6) holds. Now, let us assume that the formula is satisfied if $n = k$. Let us prove that it also holds for the value $n = k+1$. By Lemma 3, we know the sum of the combined distances obtained by the new central points and old centrals. Applying this, with the induction hypothesis, we must prove that the left hand side equals to the right hand side, so we have:

$$\frac{25k^4+45k^3+8k^2+48k}{3} + \frac{100k^3+285k^2+251k+126}{3} =$$
$$\frac{25(k+1)^4+45(k+1)^3+8(k+1)^2+48(k+1)}{3}$$
$$\frac{25k^4+145k^3+293k^2+299k+126}{3} = \frac{25k^4+145k^3+293k^2+299k+126}{3}$$

So the left hand side equals to the right hand side and the proof of the induction is complete. By the induction, it follows that formula (6) is true for all (non-negative integer value of) n. □

3.2 Sum of combined Distances between Pairs of Face Centres and Cube Vertices

Lemma 5. *Let k fcc unit cells be connected in a row and another, new, fcc unit cell be connected to the end of this row. Then the sum of combined distances between old face centres and new cube vertices plus the sum of combined* *distances between pairs formed by a new face centre and an old cube vertex is*

$$\frac{160k^3 + 648k^2 + 824k + 552}{3}. \tag{7}$$

Proof. In this proof we have to calculate the sum of total distances in the following way:

- For the sum of the distances between one of the new border points (e.g. V_{N_1}) and all old shared centres, we have

  $$(2 + 4 + 6 + \cdots + 2(k + 1)) = 2(1 + 2 + 3 + \cdots + (k + 1)) =$$

  $$\frac{2(k + 1)(k + 2)}{2} = k^2 + 3k + 2.$$

  We have to multiply it by 4 since we have 4 new border points and the formula is $4k^2 + 12k + 8$. Then, the sum of the squares of these distances is

  $4(2^2 + 4^2 + 6^2 + \cdots + (2(2k + 1))^2) = 16(1^2 + \cdots + (k + 1)^2) = \frac{16k^3+72k^2+104k+48}{3}$.

  The sum of two previous formulae is

  $$4k^2+12k+8+\frac{16k^3 + 72k^2 + 104k + 48}{3} = \frac{16k^3 + 84k^2 + 140k + 72}{3}.$$

- The sum of the distances between one of the new cube points and all side centres is: $4(3 + 5 + 7 + \cdots + (2k + 1)) = 4((k + 1)^2 - 1) = 4k^2 + 8k$; it needs to be multiplied by 4, since we have 4 new border points: the formula for this sum will be $16k^2 + 32k$.

  $$16(3^2 + 5^2 + \cdots + (2k + 1)^2) = \frac{64k^3 + 192k^2 + 176k}{3}.$$

  By summing up the two formulae, we have:

  $$16k^2 + 32k + \frac{64k^3 + 192k^2 + 176k}{3} = \frac{64k^3 + 240k^2 + 272k}{3}.$$

- The total sum of the distances between new cube vertices and new side centres is 24 (8 times 1, when the cube vertex is of the corner of the same square as the face centre is lying, e.g., V_{N_1} and C_{N_3}; plus 8 times 2, for other pairs, e.g., V_{N_1} and C_{N_5}) and the square of the distances between new cube points and new side centres is $8 \cdot 1^2 + 8 \cdot 2^2 = 40$. Further, the total sum of the distances between new cube vertices and the new shared centre (i.e., C_{N_4}) is $\sum_{i=1}^{4} d_G(V_{N_i}, C_{N_4}) = 4$. (all the 4 new cube points are neighbours of the new shared centre). Moreover, the sum of the squares of the distances between the new cube points and the new shared centre is also 4. (The total sum of distances between new cube points and new face centres is, then, $\sum_{i=1}^{4}\sum_{j=1}^{5} d_G(V_{N_i}, C_{N_j}) = 24 + 4 = 28$, actually, for each of the new four cube points it is $3\cdot 1 + 2\cdot 2$). The total combined distance between these vertices is $24 + 40 + 4 + 4 = 72$.

- The sum of distances between old cube points and the new shared centre, C_{N_4}, is

$$4(2 + 4 + 6 + \cdots + 2(k + 1)) = 4(k + 1)(k + 2) = 4k^2 + 12k + 8.$$

$4(2^2 + 4^2 + 6^2 + \cdots + 2(k + 1)^2) = 16(1 + 4 + 9 + \cdots + (k + 1)^2) = \frac{16k^3+72k^2+104k+48}{3}$.

The sum of two previous formulae is:

$$4k^2+12k+8+\frac{16k^3 + 72k^2 + 104k + 48}{3} = \frac{16k^3 + 84k^2 + 140k + 72}{3}.$$

- The sum of the distances between old cube vertices and new side centre points is given by

$4(4(3 + 5 + 7 + \cdots + (2k + 1)) + 6) = 4(4((k + 1)^2 - 1) + 1 + 1 + 2 + 2) = 16k^2 + 32k + 24$.

$4(4(3^2 + 5^2 + 7^2 + \cdots + (2k + 1)^2) + 1^2 + 1^2 + 2^2 + 2^2) = \frac{64k^3+192k^2+176k+120}{3}$.

The sum of two previous formulae is:

$16k^2 + 32k + 24 + \frac{64k^3+192k^2+176k+120}{3} = \frac{64k^3+240k^2+272k+192}{3}$.

Finally, the final formula to calculate the total sum of the combined distances between old face centre points and new cube points, plus the sum of the combined distances between the new face centre points and old cube points, plus the sum of combined distances between new cube points and new face centres, i.e., it is the sum of all previous combined distances listed by cases, i.e.,:

$$\frac{16k^3+84k^2+140k+72}{3} + \frac{64k^3+240k^2+272k}{3} + 72 + \frac{16k^3+84k^2+140k+72}{3}+$$

$$\frac{64k^3 + 240k^2 + 272k + 192}{3} = \frac{160k^3 + 648k^2 + 824k + 552}{3}.$$

Thus the proof of the lemma is finished. □

Lemma 6. *Let n fcc unit cells be connected in a row. Then the sum of combined distances between centre vertices and border vertices in this fcc grid graph is given by*

$$\frac{40n^4 + 136n^3 + 128n^2 + 248n + 24}{3}. \tag{8}$$

Proof. The proof goes by induction on n.
The base of the induction is the case $n = 1$. In this case, there are only 6 face centres, and 8 cube points. Each face centre has 4 neighbour cube vertices, and 4 other at distance 2. In this way, the combined distance between face centres and cube vertices is $6(4+4\cdot 2+4\cdot 12+4\cdot 22) = 192$ and also, formula (8) gives this value.

Let us assume that the formula satisfies if $n = k$. Let us prove that it also satisfies if $n = k + 1$. By Lemma 5, we know the sum of the new combined distances obtained between old central points and new border points (of the $(k+1)$st unit cell), between the centres of the new, $(k+1)$st unit cell and border points (of the previous k unit cells), and between the new central and the new border points (of the $(k+1)$st unit cell). Applying this, with the induction hypothesis, the following statement is needed to be proven:

In this proof, we have to prove that the left hand side equals to the right hand side:

$$\frac{40k^4 + 136k^3 + 128k^2 + 248k + 24}{3} + \frac{160k^3 + 648k^2 + 824k + 552}{3} =$$

$$\frac{40(k+1)^4 + 136(k+1)^3 + 128(k+1)^2 + 248(k+1) + 24}{3}$$

$$\frac{40k^4+296k^3+776k^2+1072k+576}{3} = \frac{40k^4+296k^3+776k^2+1072k+576}{3}.$$

Now, we proved that the left hand side equals to the right hand side. □

3.3 Sum of combined Distances between Pairs of Cube Vertices

Lemma 7. *Let k fcc unit cells be connected in a row. If a new fcc unit cell is connected to the previous k cells forming a row with $k+1$ cells, then the sum of combined distances between new and old cube vertices is*

$$\frac{64k^3 + 336k^2 + 560k + 468}{3}. \tag{9}$$

Proof. The proof goes by counting various subsums.

- Observe that the sum of distances between all pairs of the 4 new cube vertices is summed up to 12. (See Figure 2, for instance, for the distance between V_{N_1} and V_{N_2}: that is 2, i.e., $d_G(V_{N_1}, V_{N_2}) = 2$. Moreover, there are $\binom{4}{2} = 6$ such pairs of vertices). Now, we have to compute the sum of the squares of the distances: the total sum of the square of the distances between all pairs of new border vertices is $6 \cdot 2^2 = 24$. Thus, the combined distance between new cube vertices is summed up to $12 + 24 = 36$.
- Now, let us compute the sum of distances between one of the new cube vertices (e.g., V_{N_1}) and all old cube points:

  $$2 \cdot 4 + 4 \cdot 4 + 6 \cdot 4 + \cdots + 2(k+1) \cdot 4 + 1 = 4(k+1)(k+2) + 1.$$

  This result is multiplied by 4 since we have 4 new cube vertices ($V_{N_1}, V_{N_2}, V_{N_3}, V_{N_4}$). Thus, the sum of distances is

  $$4(4(k+1)(k+2)+1) = 16k^2 + 48k + 32.$$

  Next, by computing the sum of the second moment distance, we have:

  $$4(2^2 \cdot 4 + 4^2 \cdot 4 + 6^2 \cdot 4 + \cdots + (2(k+1))^2 \cdot 4 + 4 \cdot 3^2 - 4 \cdot 2^2 =$$
  $$16 \cdot 4(1^2 + 2^2 + 3^2 + \cdots + (k+1)^2) + 20 =$$
  $$\frac{16(2k+2)(k+2)(2k+3)}{3} + 20 = \frac{64k^3 + 288k^2 + 416k + 252}{3}.$$

Finally, the total combined sum is:

$$16(k+1)(k+2) + 4 + 36 + \tfrac{64k^3+288k^2+416k+252}{3} = \tfrac{64k^3+336k^2+560k+468}{3}.$$

Thus, formula (9) is obtained. □

Lemma 8. *Let n fcc unit cells be connected in a row. Then the sum of combined distances between all pairs of cube vertices is given by*

$$\frac{16n^4 + 80n^3 + 128n^2 + 244n + 108}{3}. \tag{10}$$

Proof. The proof goes by induction on n.
The base of the induction is the case $n = 1$. In this case, there are 8 corners (cube points) of the unit cell. Each pair of them has a distance 2, but pairs of opposite corners that have distance 3. The sum of distances between all pairs of these cube vertices is: $24 \cdot 2 + 4 \cdot 3 = 60$. The sum of squares of these

distances is $24 \cdot 2^2 + 4 \cdot 3^2 = 132$. Therefore, the sum of combined distances between all pairs of border vertices is 192, and also, formula (10) gives this value for $n = 1$. Now, let us assume that the formula satisfies if $n = k$. Let us prove that it also satisfies if $n = k + 1$. By Lemma 7, we know the sum of the combined distances obtained by the old and new border points. Applying this with the induction hypothesis, the next statement is needed to be proven

$$\frac{16k^4 + 80k^3 + 128k^2 + 244k + 108}{3} + \frac{64k^3 + 336k^2 + 560k + 468}{3} =$$

$$\frac{16(k+1)^4 + 80(k+1)^3 + 128(k+1)^2 + 244(k+1) + 108}{3}$$

$$\frac{16k^4 + 144k^3 + 464k^2 + 804k + 576}{3} = \frac{16k^4 + 144k^3 + 464k^2 + 804k + 576}{3}$$

So the left hand side equals to the right hand side. □

4 The Hyper-Wiener Index

Based on the results proven in the previous section, we are able to state our main result.

Theorem 9. *Let n be the number of fcc unit cells that are connected in a row. Then the formula to find Hyper-Wiener index (H) for this graph is*

$$\frac{81n^4 + 261n^3 + 264n^2 + 540n + 132}{6}. \tag{11}$$

Proof. The final formula to calculate H (see eq. 4) is the half sum of equations (6), (8) and (10). All possible distances are considered in exactly one of the Lemmas 3, 5 and 7, and then, by simple calculation the sum of those formula

$$\frac{1}{2}\left(\frac{25n^4 + 45n^3 + 8n^2 + 48n}{3} + \frac{40n^4 + 136n^3 + 128n^2 + 248n + 24}{3} + \right.$$

$$\left.\frac{16n^4 + 80n^3 + 128n^2 + 244n + 108}{3}\right) = \frac{81n^4 + 261n^3 + 264n^2 + 540n + 132}{6}.$$

The general formula to find hyper-Wiener index H for graphs of fcc unit cells that are connected in a row is proven. □

Table 1 shows some of first elements of our sequences, i.e., the values computed by equations (6), (8), (10) and (11) for some small value of n. Both W (based on Proposition 2) and H are shown in the table.

Number of unit cells(n)	1	2	3	4	5
Wiener Index W	150	536	1336	2712	4826
Equation (6)	42	296	1152	3200	7230
Equation (8)	192	920	2944	7336	15488
Equation (10)	192	668	1816	4116	8176
Hyper-Wiener index H	213	942	2956	7326	15477

Table 1: Some values of the subsums, W and H for few fcc cells in a row.

Theorem 10. *The sequence $H(n)$ can also be written in the form of a fifth-order homogenous linear recurrence with constant coefficients,*

$$H(n) = 5H(n-1) - 10H(n-2) + 10H(n-3) - 5H(n-4) + H(n-5), \quad (12)$$

when $n > 5$, and specified with values $H(1) = 213, H(2) = 942, H(3) = 2956, H(4) = 7326$ and $H(5) = 15447$.

Proof. This proof also goes by induction. The base cases, $H(n)$ with $1 \leq n \leq 5$ can be seen in Table 1.

Now, let us assume that the recurrence relation holds for each value $k < m$ for an $m \in \mathbb{N}, m > 5$. Let us prove the inheritance by computing the value for $m = k$:
$H(m) = 5H(m-1) - 10H(m-2) + 10H(m-3) - 5H(m-4) + H(m-5)$, and by the induction hypothesis we can substitute the formula for the elements of the sequence on the right hand side:

$$\begin{aligned}
H(m) = 5 & \ \tfrac{81(m-1)^4+261(m-1)^3+264(m-1)^2+540(m-1)+132}{6} \\
-10 & \ \tfrac{81(m-2)^4+261(m-2)^3+264(m-2)^2+540(m-2)+132}{6} \\
+10 & \ \tfrac{81(m-3)^4+261(m-3)^3+264(m-3)^2+540(m-3)+132}{6} \\
-5 & \ \tfrac{81(m-4)^4+261(m-4)^3+264(m-4)^2+540(m-4)+132}{6} \\
+ & \ \tfrac{81(m-5)^4+261(m-5)^3+264(m-5)^2+540(m-5)+132}{6} \\
= & \tfrac{5\cdot 81(m^4-4m^3+6m^2-4m+1)-10\cdot 81(m^4-8m^3+24m^2-32m+16)}{6} \\
+ & \tfrac{10\cdot 81(m^4-12m^3+54m^2-108m+81)}{6} \\
+ & \tfrac{-5\cdot 81(m^4-16m^3+96m^2-256m+256)+81(m^4-20m^3+150m^2-500m+625)}{6} \\
+ & \tfrac{5\cdot 261(m^3-3m^2+3m-1)-10\cdot 261(m^3-6m^2+12m-8)+2610(m^3-9m^2+27m-27)}{6} \\
+ & \tfrac{-5\cdot 261(m^3-12m^2+48m-64)+261(m^3-15m^2+75m-125)}{6} \\
+ & \tfrac{5\cdot 264(m^2-2m+1)-10\cdot 264(m^2-4m+4)+10\cdot 264(m^2-6m+9)}{6} \\
+ & \tfrac{-5\cdot 264(m^2-8m+16)+264(m^2-10m+25)}{6}
\end{aligned}$$

$$+\frac{5\cdot 540(m-1)-10\cdot 540(m-2)+10\cdot 540(m-3)-5\cdot 540(m-4)+540(m-5)}{6}+\frac{132}{6}.$$

Further,

$$\begin{aligned}H(m) &= \frac{81m^4+(81\cdot(-5\cdot 4+10\cdot 8-10\cdot 108+5\cdot 256-20)+261)m^3}{6}\\ &+\frac{(81\cdot(5\cdot 6-10\cdot 24+10\cdot 54-5\cdot 96+150)+261\cdot(-5\cdot 3+10\cdot 6-10\cdot 9+5\cdot 12-15)+264)m^2}{6}\\ &+\frac{(81\cdot(-5\cdot 4+10\cdot 32-10\cdot 108+5\cdot 256-500)+261\cdot(5\cdot 3-10\cdot 12+10\cdot 27-5\cdot 48+75))m}{6}\\ &+\frac{(264\cdot(-5\cdot 2+10\cdot 4-10\cdot 6+5\cdot 8-10)+540)m}{6}\\ &+\frac{81\cdot(5\cdot 1-10\cdot 16+10\cdot 81-5\cdot 256+625)+261\cdot(-5\cdot 1+10\cdot 8-10\cdot 27+5\cdot 64-125)}{6}\\ &+\frac{264\cdot(5\cdot 1-10\cdot 4+10\cdot 9-5\cdot 16+25)+540\cdot(-5\cdot 1+10\cdot 2-10\cdot 3+5\cdot 4-5)+132}{6}\\ &= \frac{81m^4+261m^3+264m^2+540m+132}{6}.\end{aligned}$$

That is exactly the formula (11) for m. Since the inheritance is proven, the statements of the theorem is proven. □

5 Conclusions

Theoretical work on various lattices and grids has various connections to digital and discrete geometry, graph and lattice theory, crystallography and various theoretical and applied fields in physics and chemistry. After the success of Wiener-index, several other important topological/geometrical indices are defined for various graph structures; one of those is the hyper-Wiener index. In this paper, the face-centred cubic lattice is analysed, especially, when a finite number of unit cells are placed next to each other at a line. We have presented and proved formula for the computation of hyper-Wiener index for these graphs. There are several ways to continue the line of the research that we have just started here:

- One can compute other topological indices, e.g., Szeged or Zagreb indices [7] for these graphs.
- One can extend the results to two and three dimensional rectangles and blocks of unit cells.
- Wiener index and hyper-Wiener index may be further generalised including higher moment of the distances.
- Finally, having results on various crystal structures, the results could be compared to various physical and chemical properties of the crystals belonging to these classes. We believe that hyper-Wiener index is related to some of these properties and thus these indices can have direct applications.

Acknowledgements

The support of the Deanship of Scientific Research at Al-Quds Open University is gratefully acknowledged.

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