Graph Indices on Grids

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ABSTRACT

The Wiener index of a graph, known as the “sum of distances” of a connected graph, is the first topological index used in chemistry to sum the distances between all unordered pairs of vertices of a graph. Wiener index, or sometimes called Wiener number, of a molecular graph correlates physical and chemical characteristics of graphs, and has been studied for various kinds of graphs. In this thesis, we derived mathematical formulas to compute Wiener index and hyper-Wiener index for body-centered cubic grid and face-centered cubic grid. In the body-centered cubic graph, the lines of unit cells of the body-centered cubic grid are used. These graphs contain center points of the unit cells and other vertices, called border vertices. Closed formulas are obtained to calculate the sum of shortest distances between pairs of border vertices, between border vertices and centers and between pairs of centers. Based on these formulas, their sum, the Wiener index and hyper-Wiener index of body-centered cubic grid with unit cells connected in a row are computed. Some relationships between formulas and integer sequences are also presented.

In face-centerd cubic grid, the graphs of lines of unit cells of the face-centered cubic grid are investigated. The face-centered cubic unit cell is a cube (all sides have the same length and all faces are perpendicular to each other) with an atom at each corner of the unit cell called border points and an atom situated in the middle of each face of the unit cell called face central points. Closed formulas are obtained to calculate the sum of shortest distances between pairs of border points, between border points and centrals and between pairs of centrals. Based on these formulas,

their sum, the Wiener index and hyper-Wiener index of face-centered cubic grid with unit cells connected in a row graph is computed.

Keywords: Wiener index, body-centered cubic grid, face-centered cubic grid, hyper-Wiener index, shortest paths, non-traditional grids, combinatorics.

ÖZ

Bir grafın mesafeler toplamı olarak bilinen Wiener indeksi, kimdaya sırasız düğüm çiftleri arasındaki mesafeler toplamını hesaplamak için kullanılan ilk topolojik indekstir. Moleküler grafın bir çok graf türü için irdelenmiş olan ve Wiener sayısı olarak da bilinen Wiener indeksi grafın fiziksel ve kimyasal özelliklerini ilişkilendirir. Bu tezde gövde-merkezli grafın birim hücrelerinin kenarlarını kullanarak gövde-merkezli ve yüzey-merkezli kübik grafın Wiener indeksi ve hiper-Wiener indeksinin hesaplanması için formül geliştirilmiştir. Bunun yanı sıra yüzey-merkezli kübik şebekelerde birim hücre dizileri biçiminde olan graflar irdelenmiştir. Yüzey-merkezli kübik birim hücre, köşeleri sınır noktaları da denilen çekirdeklerden oluşan bir küpdür. Sözkonusu graflar birim hücreleri merkez düğümlerini ve sınır düğümlerini içermektedir. Bu bağlamda önerilen formüller uygulanarak sınır düğümleri çiftleri, sinir ve merkez düğüm çiftleri ve merkez düğüm çiftleri arasındaki en kısa yollar toplamı hesaplanabilmektedir. Sözkonusu formüller ve tamsayı dizileri arasında bazı ilişkiler de bu tezde irdelenmiştir.

Anahtar Kelimeler: Wiener endeksi, gövde-merkezli kübik grid, yüzey-merkezli kübik grid, hiper-Wiener endeksi, kısa yollar, Geleneksel olmayan grid, kombinatoriks.

DEDICATION

To My Mother (God bless her soul)

ACKNOWLEDGMENT

I would like to express my special appreciation and thanks to Dr. Benedek Nagy for his continuous support and guidance of my PhD study and research. His invaluable supervision and guidance, help me to complete my dream.

I would like to thank all the academic staff in the Department of Art and Science, Eastern Mediterranean University, for their help and support with various issues during the study and I am grateful to all of them. I am also obliged to Prof. Dr. Younes Amro, president of Al-Quds Open University for his help and support during my study. My friends have helped me through these difficult years, I would like to thank them all.

Last but not the least, I would like to thank my family for their help and support. I dedicate this thesis to them as an indication of their significance in this study as well as in my life.

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LIST OF SYMBOLS/ABBREVIATIONS

WI	Wiener Index
WW	Hyper-Wiener index
bcc	Body-centered cubic
fcc	Face-centered cubic
QSAR	Quantitative Structure Activity Relationships
QSPR	Quantitative Structure Property Relationships
G	Graph
P	Path
E	Edge
V	Vertex
NaCl	Sodium Chloride
TW	Terminal Wiener index
SEMS	Super Edge-magic Sequence
LHS	Left Hand Side
RHS	Right Hand Side

Chapter 1

INTRODUCTION

1.1 Introduction

Various crystals can be found in the nature; most of them are described by crystal systems (3D graphs). Graph theory is used in almost every field of science and it is also heavily used in practice for simulations and engineering solutions. Graph theory is now playing an important role not only in Mathematical researches, but in Electrical Engineering, Computer Programming, Networking, Geography, Crystallography, etc. The atoms/molecules/ions of most of the crystals use graphs with regular, periodic structures. Digital geometry deals with the description of these regular tessellations. Digital geometry has also close connection to image processing and computer graphics [18]. One of the main directions of research of digital geometry deals with descriptions and applications of non-traditional grids [23,31,32,33]. (Square and cubic grids are counted as traditional grids, since they are the most usual in mathematics and engineering.) Non-traditional 3D grids, for instance, body-centered cubic (bcc), face-centered cubic (fcc) and diamond cubic grids play an important role in physics and chemistry, as well, since various materials have these crystal structures, and the properties of the materials are closely related to their structures.

1.2 Motivation

Graph theory is the study of graphs, and it is an important part of discrete mathematics. It is being directly used in fields such as communication networks, biochemistry (genomics), computer science such as algorithms and computation. One of the robust combinatorial ways found in graph theory has been used to prove basic results in other fields of pure mathematics. In particular, graph theory is the study of graphs containing nodes and edges. It involves the ways in which sets of points, called vertices, can be connected by lines or arcs, called edges.

Topological index, sometimes also known as a graph-theoretic index, is a numerical invariant of a chemical graph [25]. Particular topological indices include but not limited to molecular topological index, the Balaban index, Harary index, and Wiener index. Topological indices are used as simple numerical descriptors in comparing physical, chemical or biological parameters of molecules in Quantitative Structure Property Relationships (QSPR) and in Quantitative Structure Activity Relationships (QSAR) [3]. There are different studies about topological indices, one of the most widely known topological descriptor is the Wiener Index (*WI*). In fact, it is being studied consequently for various graphs over the last decades after being introduced by chemist Harold Wiener about 70 years ago to illustrate relationship between physicochemical properties of organic compounds and the topological structure of their molecular graphs [37]. *WI* is a distance-based graph invariant, used as one of the structure descriptors for predicting physicochemical properties of organic compounds [30].

WI is a graph invariant that belongs to the molecular structure descriptors, called topological indices. These indices are widely used by chemists to design molecules with desired properties. In the initial applications, the *WI* is employed to anticipate physical parameters such as boiling points of the paraffins [37]. Other measurable physical quantities, e.g., molar volumes, heats of vaporization and molar refractions of various molecules can be characterized in a similar manner. The first mathematical definition of *WI* is based on the concept of graph theoretical distance. Topological indices are designed and used to assign a number to each (given type) molecular graph by some measure [37]. *WI* is used to study the relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds. Mathematically these systems are usually hexagonal systems [9]. The *WI* is, generally, defined as the sum of the shortest distances between every pair of vertices of *G*. For molecules, in general, *WI* measures how compact a molecule is for its given weight. The molecule is more compact if its *WI* value is less. Wiener, originally, presented the concept 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 [37]. However, the index named after him, the *WI* is defined as

$$WI(G) = \frac{1}{2}\sum_{u,v\in V(G)} d_G(u,v) \tag{1.1}$$

i.e., 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* [20]. *WI* measures how compact a molecule is for its given weight. The molecule is more compact if its *WI* value is less.

Randic [26], proposed hyper-Wiener index (*WW*) for trees and this newer concept was extended to all connected graphs by Klein, Lukovits and Gutman in [17]. *WW* is also used as a structure-descriptor for detecting physicochemical characteristics of organic compounds. It is one of the recent distance-based graph invariants, often used in different fields such as agriculture, pharmacology, environment-protection, etc. [5,16,38]. The formula below suggests that *WW* clearly encodes the "compactness" of a structure. Furthermore, the squared term gives relatively more weight to extended structures, and *WW* should therefore be 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:

$$WW(G) = \frac{1}{2} WI(G) + \frac{1}{4} \sum_{u,v \in V(G)} d_G^2(u,v) \tag{1.2}$$

where *WI*(*G*) is the Wiener index of the graph *G*. Actually, the *WW* is the average of the *WI* and the (unnormalized) second moment distance.

1.3 Thesis Contribution

In this thesis, we investigated, studied and calculated *WI* and *WW* for different types of molecular graphs. Theses graphs include body-centered cubic bcc grids and face-centered cubic fcc grids. These grids are the most usual crystal structures.

For the bcc grid graph, the lines of unit cells of the bcc grid are used. These graphs contain center points of the unit cells and other vertices, called border vertices. Closed formulas are obtained to calculate the sum of shortest distances between pairs of border vertices, between border vertices and centers and between pairs of centers. Based on these formulas, their sum, the *WI* and *WW* of bcc grid with unit cells connected in a row graph is computed. Some relationships between formulas and integer sequences are also presented.

For the fcc grid, the graphs of lines of unit cells of the fcc grid are investigated. Its graphs contain central points of the unit cells and other vertices, called border points. Closed formulas are obtained to calculate the sum of shortest distances between pairs of border points, between border points and centrals and between pairs of centrals. Based on these formulas, their sum, the *WI* and *WW* of fcc grid with unit cells connected in a row graph is computed.

The work of this thesis is based on the following publications:

- Mujahed, H., Nagy, B. (2015). Wiener index on Lines of Unit Cells of the body-centered cubic Grid. ISMM 2015: 12th International Symposium on Mathematical Morphology and Its Applications to Signal and Image Processing, LNCS 9082, 597–606.
- Mujahed, H., Nagy, B. (2016). Wiener index on rows of unit cells of the face-centred cubic lattice. Acta Cryst. A72, pp. 243–249.

1.4 Thesis Outline

This thesis is organized as follows: Chapter one gives and presents general introduction about graph theory, molecular graph *WI* and *WW*. A concise literature review about previous studies which involve algorithms and mathematical methods to compute *WI* is investigated in chapter two. Chapter three contains detailed description about bcc grid and mathematical formulas to calculate *WI* and *WW* for lines of unit cells of the bcc grid. Chapter four contains detailed description about fcc grids and mathematical formulas to calculate *WI* and *WW* on rows of unit cells of the face-centered cubic grid. Finally in chapter five the conclusions for this work are presented, and some possible future work are mentioned.

Chapter 2

LITERATURE REVIEW AND PRELIMINARIES

2.1 Introduction

We will start this section by basic definitions and fundamental concepts about graphs:

- A graph G is an ordered pair of disjoint sets (V, E) such that E is a subset of the set of unordered pairs of V. The set V is the set of vertices and E is the set of edges [4].

- Often, we label the vertices with letters (for example: a, b, c, etc.; or v_1, v_2, v_3, etc.) or numbers (for example 1, 2, 3, etc.) (See Figure 1).

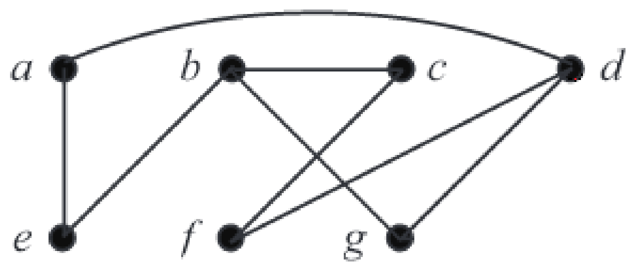


Figure 1: A visual representative of graph G

- For a graph G, we denote by $V(G)$ and $E(G)$ its sets of vertices and edges, respectively. An edge (a, e) is said to join the vertices a and e and is denoted by ae. Thus ae and ea mean exactly the same edge, the vertices a and e are the end vertices of this edge.

- Two vertices b and c are adjacent if they are connected by an edge, in other words, (b, c) is an edge.
- An edge of the form (a, a) is a loop.
- The edges indicate a two-way relationship, in that each edge can be traversed in both directions.
- A path in the graph is a sequence of distinct vertices $v_1, v_2, v_3, \ldots, v_n$ such that (v_i, v_{i+1}) is an edge for each $i=1,\ldots,n-1$.
- The length of a path P, denoted $|P|$, is the number of its edges [4].
- A graph G is connected if given any two vertices in this graph, there is a path from one vertex to another.
- The distance between two vertices a and b denoted by $d_G(a, b)$, is the length of shortest path connected a and b.
- Undirected graphs have edges that do not have a direction. (See Figure 1).
- Simple graph, is an undirected graph containing no graph loops or multiple edges.

In this thesis, all graphs are simple, undirected and connected without loops or multiple edges.

A topological representation of a molecule is called molecular graphs. 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. To determine molecular graph of some chemical compound, the molecular graph invariants, called topological indices could be used too. The most important use of these topological indices are designed basically by transforming a molecular graph into a number. By these numbers some of the measured properties of the molecules can be predicted [37]. Not only molecules can be represented by graphs: there are some elements that form atomic grid, e.g. carbon and silicon. In a similar manner, crystals formed by ions can be modelled and measured by graphs underlining their structure, see, e.g., [1]. Moreover, in other crystals, such as in metals, the atoms (cations) are placed according to a well-defined arrangement. The most usual arrangements for metals are the body-centered and the face-centered cubic grids. In body-centered cubic grid (bcc grid, in short) the atoms are located in a cubic structure and, additionally, there is an atom in the center of each unit cube. The face-centered cubic grid (fcc grid, in short) has unit cells that are cubes with an atom at each corner of the unit cells and an atom situated in the middle of each (square) face of the unit cells.

2.2 General Review

A topological index is a numeric quantity associated with chemical constitution and the correlation of chemical structure with various chemical and physical properties of a molecule. Topological indices are mathematically derived in various ways from the structural graph of a molecule. One of the most important topological index is *WI*. *WI* is employed to predict heats of vaporization, molar volumes, boiling points and molar refractions of alkanes. Alkanes are the simplest organic molecules. Alkanes are chemical compounds that include carbon (*C*) and hydrogen (*H*) atoms, so they are also called hydrocarbons. In chemistry concepts and theory, distance-based molecular structure descriptors are used for modeling pharmacologic, biological, physical, and other properties of chemical compounds.

To our basic knowledge and investigation, there is no direct and unified technique to compute *WI* of graphs. The problem to find a general formula or a technique to calculate *WI* for graphs is still open. Most of the work in the field of calculating *WI* depend on special types of graphs. In our work, we are also contributing the field with calculations on specific graphs.

The concept of a *WI* which is introduced by Wiener in 1947 [37] open the doors for more research area in the field of topological indices. Many methods, mathematical equations and algorithms for computing the *WI* of a graph were proposed in the chemical, mathematical and related computational literature.

In [7], the authors presented a linear time algorithm to compute *WI* of given benzenoid graph *G*. The main idea of the algorithm depends on an isometric embedding concept of graph *G* into the Cartesian product of three trees, combined with the notion of the *WI* of vertex-weighted graphs.

In [17] the authors work in order to extend the definition of Randic for *WW* in two different fashions so as to be suitable and applicable for any connected structure. The formula provides an easy method to calculate the *WW* for any graph.

In [5], the theoretical approach for computing *WW* discussed. The authors in this research consider three different methods for calculating the *WW* of molecular graphs: the cut method, the method of Hosoya polynomials and the interpolation method. The authors discussed drawbacks, advantages and get several new closed-form expressions for the calculation of *WW* for infinite families of molecular graphs.

In [16], an algorithm to compute the *WW* of benzenoid hydrocarbons is described, based on the consideration of pairs of elementary cuts of the corresponding benzenoid graph *G*.

In [1], the *WI* of chemical structures such as sodium chloride *NaCl* and benzenoid graph computed without using distance matrix. An efficient method of computing *WI* of chemical structures such as honeycomb, benzenoid and sodium chloride graph.

In [13], a method for evaluating the sum of all distances, known as the *WI*, of the zig-zag nanotubes and general square connected layers is presented.

In [36], formula for the calculation of the *WI* of pericondensed benzenoid graphs made up from three rows of hexagons of various lengths is given. In order to verify the formula, a program, written in a Pascal-based pseudocode that calculates *WI* of a benzenoid system from its ring-matrix is used.

In [6], an algorithm is presented for the generation of molecular graphs with a given value of the *WI*.

In [12], the terminal Wiener index (*TW*) is a newer molecular-structure descriptor. And there is only a limited number of its mathematical properties were established so far. Results on terminal *WI* of thorn graphs are presented.

In [19], the authors developed a method to calculate the *WI* of some kinds of molecular graphs. These graphs are three regular plane tessellations composed of the same kind of regular polygons (triangular, square and hexagonal). The new technique in this paper could be used to compute *WI* for more chemical graphs.

In [8], explicit formula for *WI* of hypercubes and their corresponding Euclidean graph is given. Also the method used to compute and express completely the explicit mathematical formulas for *WI* for hypercubes and Euclidean graph of *n*-dimensional hypercubes which has applications in mathematical chemistry.

In [10], a modification of the *WI* which properly consider the symmetry of a graph is proposed. The explicit formula for the modified *WI* of special case (type) of graphs are founded and compared with their standard *WI*.

In [11], the concept of line graph has various applications in physical chemistry. In that paper, the authors obtained the *WI* of line graphs and some other classes of graphs.

In [34], MATLAB algorithm for finding the *WI* of the molecular graph was presented. MATLAB program is written to compute *WI* based on adjacency matrix as input. In this kind of MATLAB calculations, the only difficult thing is how to find the adjacency matrix easily for graph *G*.

In [27], the result on *WW* of amalgamation of complete graph with common vertex and Amalgamation of cyclic graph with common edge is proved. This paper also investigated the three methods for calculation of the *WW* of molecular graphs which include cut method, distance formula and the method of Hosaya polynomials.

In [14], *WW* of the Cartesian product, composition, join and disjunction of graphs are calculated. These results are used to compute the *WW* of C_4 nanotubes and some other graphs.

In [28], the authors proved some general results on *WW* of thorny-complete graphs.

In [35], *WI* for some molecular graph is being calculated in two different ways: the first way based on a new method using Super Edge-magic Sequence (SEMS) and the second way based on different approach for existing method, using minimal spanning tree at each vertex. This approach will help to change the chemical formula into sequence.

2.3 Preliminaries

In previous sections, we have already provided the concepts of graphs. Now we recall those grid graphs we are working on.

2.3.1 Body-Centered Cubic Grid

By adding a grid point in the center of each cube with vertices on grid points in a cubic grid, a body-centered cubic (bcc) is obtained. The bcc unit cell is a cube (all sides are of the same length and all faces sharing a corner are perpendicular to each other) with an atom at each corner of the unit cell and an atom in the center of the unit cell [15, 31, 32]. Each of the corner atoms is the corner of another cube, thus atoms in the corner are shared among eight unit cells. It is said that bcc unit cell has a coordination number of 8 and a bcc unit cell consists of a net total of two atoms; one in the center and eight eighths from corner atoms. Some of the materials that have a bcc grid structure include lithium, sodium, potassium, chromium, barium, vanadium, alpha-iron and tungsten. Metals which have a bcc grid structure are usually harder and less malleable than close-packed (e.g., fcc grid structured) metals such as gold. When the metal is distorted, the planes of atoms must slip over each other, and this process is harder in the bcc unit cell structure [15]. In Figure 2 a bcc unit cell is shown, moreover, the closest atoms are connected to each other. Cesium chloride and some other salts use also the same structure in their crystals having one type of atoms in the corners of a unit cell and the other type in the center. Thus, the neighbour relation in these salts contains only atoms (i.e., ions) of different kinds: an anion (e.g., Cl^{-}) and a cation (e.g., Cs^{+}). In salts, actually, the ionic bonds can be represented by connecting the neighbour ions. Connecting the closest atoms in a bcc grid, its usual graph-representation is obtained.

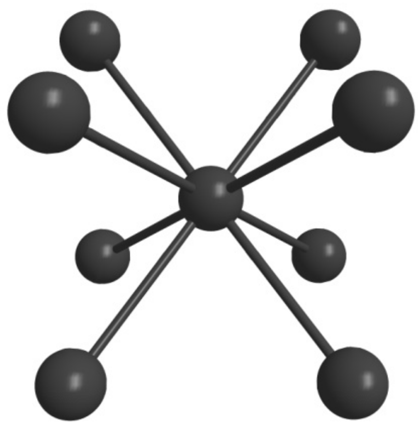
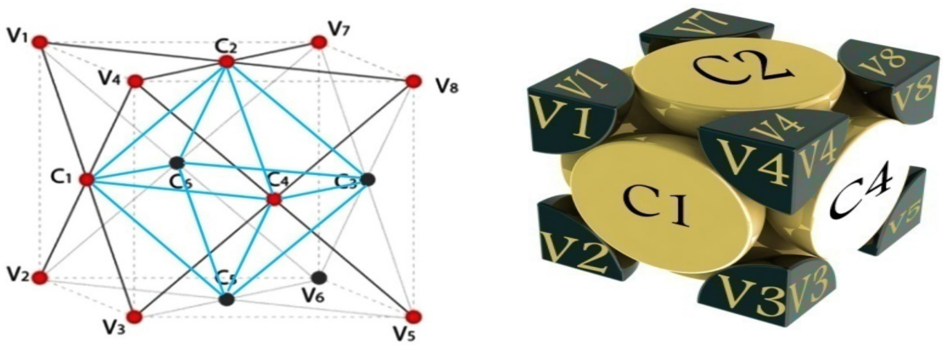


Figure 2: A unit cell of body-centered cubic grid showing the neighbour relation of the atoms

2.3.2 Face-Centered Cubic Grid

Face-centered cubic (fcc) grid consists of unit cells with an atom at each corner of cube and an atom in the center of each face of the cube. The fcc unit cell structure is shown in Figure 3. In this structure atoms are arranged at the eight corners and at the centers of the six faces of a cube.

The fcc unit cell is a repeating unit in a cubic closest-packed structure. In fact, Figure 3 (b) explains why the structure is known as cubic closest-packed. Metals with the fcc unit cell structure include: aluminium, copper, nickel, gold and silver. Due to their structure it is relatively easy to work with these metals (comparing to other metals with bcc grid structure).



(a) (b)

Figure 3: A unit cell of face-centered cubic (fcc) grid showing the neighbour relation of the atoms (solid lines) (a), and fcc grid close-packing with spheres (b)

Chapter 3

WIENER INDEX AND HYPER-WIENER INDEX ON LINES OF UNIT CELLS OF THE BODY-CENTERED CUBIC GRID

3.1 Wiener Index for a Row of bcc Unit Cells

In this thesis, we are using graphs that represent a row of unit cells of the bcc grid (i.e., the dimension of our space is $n\times1\times1$ unit cells). We use the terms center points and border points/vertices for the points located on a center of a unit cell and on the corner of a cell, respectively.

In this sections we present our results. In the next subsections some subsums are computed that are needed later on. We start with a straightforward result:

Lemma 3.1. Let n be the number of bcc unit cells connected in a row, the number of vertices V in this graph is given as follows (the first term gives the number of border vertices, the second term is the number of center vertices):

$$|V| = (4n+4)+n. \tag{3.1}$$

The *WI* is computed as the sum of the distances of all unordered pairs of vertices. In our graphs we have two types of vertices. Thus, in our graphs, *WI* can be computed as the sum of the following three subsums:

- sum of the distances between unordered pairs of centers,
- sum of the distances between pairs of centers and border vertices, and
- sum of the distances between unordered pairs of border vertices.

In the next three subsections these subsums are considered.

3.1.1 Sum of Distances between Center Points

Lemma 3.2. Let k bcc unit cells be connected in a row and, 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 all distances between the new center and all old centers is

$$k(k+1)\,. \tag{3.2}$$

Proof: The distances of the new center C_N to the old centers are: $d_G(c_N,c_1)=2$, $d_G(c_N,c_2)=4$, ..., $d_G(c_N,c_k)=2k$, therefore the sum of the even numbers from 2 to $2k$ is needed, and it gives the result shown in (3.2). (See also Figure 4.) □

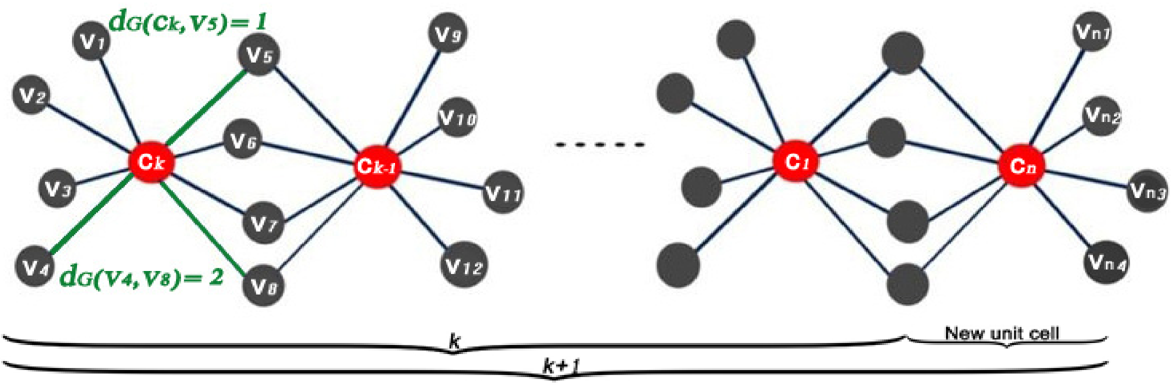


Figure 4: k bcc unit cells connected in a row with a new unit cell attached the end of the row

Lemma 3.3. Let n bcc unit cells be connected in a row. Then the sum of all distances between center vertices in this bcc grid graph is given by

$$\frac{n^3-n}{3} \tag{3.3}$$

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 1 center, and thus there is no distance to sum up, consequently the sum has value 0, and the formula 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 3.2, we know the sum of the distances obtained by the new center and old centers. Applying this, with the induction hypothesis we get

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

The proof of the induction is complete. By the induction, it follows that formula (3.3) is true for all (non-negative integer value of) n. □

3.1.2 Sum of Distances between Centers and Border Vertices

Lemma 3.4. Let k bcc unit cells be connected in a row and let a new bcc unit cell be connected to the end of this row. Then the sum of the distances between old centers and new border vertices plus the sum of the distances between the new center and old border vertices is

$$8(k+1)^2. \tag{3.4}$$

Proof: Observe that the 4 new border vertices (see also Figure 4, they are on the right) are connected to the new center and some of the old border vertices are also connected to the new center. We need to count the sum of the distances between the 4 new border vertices and the new and old centers, and between the old border vertices and the new center. The sum of these distances can be written in the form

$$\underbrace{4\cdot1+4\cdot3+4\cdot5+4\cdot7+\ldots+4(2k+1)}_{(\textit{new vertices to all centers})}+\underbrace{4\cdot1+4\cdot3+4\cdot5+4\cdot7+\ldots+4(2k+1)}_{(\textit{old vertices to new center})}=$$
$$=2(4\cdot1+4\cdot3+4\cdot5+4\cdot7+\ldots+4(2k+1))=8(1+3+5+7+\ldots+(2k+1))=8(k+1)^2. \quad □$$

Lemma 3.5. Let n bcc unit cells be connected in a row. Then the sum of all distances between center vertices and border vertices in this bcc grid graph is given by

$$2\binom{2n+2}{3}. \tag{3.5}$$

Proof: The proof goes by induction on n.

The base of the induction is the case $n = 1$. In this case, there is only 1 center, and it is connected to every of the 8 corners (border points) of the unit cell having unit distances. The sum is 8, and also, formula (3.5) 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 3.4, we know the sum of the new distances obtained between old centers and new border vertices (of the (k+1)st unit cell), between the (k+1)st center and border vertices (of the previous k unit cells), and between the new (k+1)st center and the new border vertices (of the (k+ 1)st unit cell), see Figure 4. Applying this, with the induction hypothesis gives the following statement that is needed to be proven:

$$2\binom{2k+2}{3}+8(k+1)^2 = 2\binom{2(k+1)+2}{3} = 2\binom{2k+4}{3}.$$

By using the definition of the Binomial coefficients and applying mathematical simplifications, we get

$$\frac{(2(k+1))!}{3(2(k+1)-3)!}+8(k+1)^2 = \frac{(2(k+2))!}{3(2(k+2)-3)!}.$$

Further, multiplying both sides by 3,

$$\frac{(2k+2)!}{(2k-1)!}+24(k+1)^2 = \frac{(2k+4)!}{(2k+1)!}.$$

Now, our aim is to prove that the left hand side (LHS) equals to the right hand side (RHS)

$$\frac{(2k+2)(2k+1)(2k)(2k-1)!}{(2k-1)!}+24(k+1)^2=\frac{(2k+4)(2k+3)(2k+2)(2k+1)!}{(2k+1)!}.$$

Then, we have

$$8k^3+36k^2+52k+24=8k^3+36k^2+52k+24. \qquad \square$$

Observe that equation (3.5) can also be written in the form $\frac{8n^3+12n^2+4n}{3}$.

3.1.3 Sum of Distances of Border Vertices

Lemma 3.6. Let k bcc unit cells be connected in a row. If a new bcc unit cell is connected to the previous k cells forming a row with k+1 cells, then the sum of all distances between new and old border vertices is

$$16(k+1)(k+2)+12. \qquad (3.6)$$

Proof: Observe that the sum of distances between all pairs of the 4 new vertices is 12. (See Figure 4, 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 $\binom{4}{2}=6$ pairs).

Now, let us compute the distance between one of the new border vertices (e.g., v_{N_1}) and all old border vertices:

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

This result is multiplied by 4 since we have 4 new vertices (v_{N_1}, v_{N_2}, v_{N_3}, v_{N_4}). Thus we have:

$$16(k+1)(k+2).$$

Finally, the total sum of distances between all new and old border vertices is given by the sum of the previous two values:

$$16(k+1)(k+2)+12.$$

Thus, formula (3.6) is obtained. □

Lemma 3.7. Let *n* bcc unit cells be connected in a row. Then the sum of all distances between pairs of border vertices is given by

$$\frac{16(n+1)^3+20(n+1)}{3}. \tag{3.7}$$

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 (border points) of the unit cell. Each pair of them has a distance 2 (by connecting them through the center), therefore the sum of distances between all pairs of border vertices is 56, and also, formula (3.7) gives this value.

Now, let us assume that the formula satisfies if $n=k$. Let us prove that it also satisfies if $n=k+1$. By Lemma 3.6, we know the sum of the distances obtained by the old and new border vertices. Applying this, with the induction hypothesis gives the statement that is needed to be proven

$$\frac{16(k+1)^3+20(k+1)}{3}+(16(k+1)(k+2)+12)=\frac{16(k+2)^3+20(k+2)}{3}.$$

The result can be proven by the following mathematical simplifications/modifications starting from the LHS. It equals to

$$\frac{16(k+1)^3+20(k+1)+48(k+1)(k+2)+36}{3}=\frac{16(k+2-1)^3+(k+1)(20+48(k+2))+36}{3}=$$

$$=\frac{16((k+2)^3-3(k+2)^2+3(k+2)-1)+(k+1)(20+48(k+2))+36}{3}=$$

$$=\frac{16(k+2)^3-48(k+2)^2+48(k+2)-16+20(k+1)+48(k+1)(k+2)+36}{3}=$$

$$=\frac{16(k+2)^3+(k+2)(-48(k+2)+48+48k+48)+20(k+1)+20}{3}=$$

$$=\frac{16(k+2)^3+20((k+1)+1)}{3}=\frac{16(k+2)^3+20(k+2)}{3}.$$

This is exactly the formula on the RHS. □

3.1.4 Sum of All Distances: The Main Formula

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

Theorem 3.1. Let n be the number of bcc unit cells that are connected in a row. Then the formula to find WI for this graph is:

$$WI(n)=\frac{25n^3+60n^2+71n+36}{3}. \tag{3.8}$$

Proof: The formula is the sum of equations (3.3), (3.5) and (3.7). All possible distances are considered in exactly one of the lemmas 3.3, 3.5 and 3.7, and then, by simple calculation the sum of those formulas,

$$\frac{16(n+1)^3+20(n+1)}{3}+2\binom{2n+2}{3}+\frac{n^3-n}{3},$$

Can be written in the form of equation (3.8). □

Using formula (3.8) one can calculate WI for graph of bcc unit cells connected in a row, as we will present some examples later in this chapter.

3.2 Hyper-Wiener Index for bcc Grid connected in a Line

WI, WW and other indices are introduced to reflect certain structural properties of organic molecules. There are several studies contributed to determine the distance-based index of special molecular graphs. The WW of acyclic graphs was introduced by Milan Randic in 1993 [26]. Then Klein, Lukovits and Gutman [17], generalized

Randic's definition for all connected graphs, as a generalization of the *WI*. We recall equation (1.2) in chapter one, and make small transformation on the formula computing *WW*:

$$WW(G)=\frac{1}{2}\left(WI(G)+\frac{1}{2}\sum_{u,v\in V(G)}d_G^2(u,v)\right)=\frac{1}{2}\left(\frac{1}{2}\sum_{u,v\in V(G)}d_G(u,v)+\frac{1}{2}\sum_{u,v\in V(G)}d_G^2(u,v)\right),\text{ and thus}$$

$$WW(G)=\frac{1}{4}\sum_{u,v\in V(G)}\left(d_G(u,v)+d_G^2(u,v)\right), \tag{3.9}$$

Where $d_G(u,v)$ is the distance between the two vertices in the graph, and $WI(G)$ is the normal *WI* proposed by Wiener in 1947. In (3.9), to compute *WW* the distance and second moment distance of the pairs of nodes are summed up. In the following three subsections we will compute the sums between various types of vertices. Actually, to compute *WW* the value $\left(d_G(u,v)+d_G^2(u,v)\right)$ is needed for each unordered pair of vertices u and v. For simplifying our notions, we refer for sums of values $\left(d_G(u,v)+d_G^2(u,v)\right)$ as sums of combined distances.

3.2.1 Sum of Combined Distances between Pairs of Centers

Let us start by the sum of combined distances between center points.

Lemma 3.8. Let k bcc 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 the new center and all old centers is

$$\frac{4k^3+9k^2+5k}{3}. \tag{3.10}$$

Proof: The distances of the new center C_N to the old centers are: $d_G(c_N,c_1)=2$, $d_G(c_N,c_2)=4,\ldots,d_G(c_N,c_k)=2k$, therefore the sum of the even numbers from 2 to $2k$ is needed plus the sum of their squares: $(2)^2$, $(4)^2$ up to $(2k)^2$ is needed also in order to have the result shown in (3.10). (See also Figure 4.) Thus, to explain in detail, we have

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

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

The sum of two previous equations is: $k(k+1) + \frac{4(k^2 + k)(2k+1)}{6} = \frac{4k^3 + 9k^2 + 5k}{3}$.

Thus the proof of the lemma is finished. □

Lemma 3.9. Let *n* bcc unit cells be connected in a row. Then the sum of combined distances between center vertices in this bcc grid graph is

$$\frac{n^4 + n^3 - n^2 - n}{3}. \tag{3.11}$$

Proof: The proof goes by induction.

The base of the induction is the case $n = 1$. In this case, there is only 1 center, and thus there is no distance to sum up, consequently the sum has value 0, and the formula holds. Now, let us assume that the formula holds up to a value k. Let us prove that it also holds for the value k+1. By Lemma 3.8, we know the combined distance obtained by the new center and old centers. Applying this, with the induction hypothesis gives

$$\frac{k^4 + k^3 - k^2 - k}{3} + \frac{4k^3 + 9k^2 + 5k}{3} = \frac{(k+1)^4 + (k+1)^3 - (k+1)^2 - (k+1)}{3}.$$

$$\frac{k^4 + 5k^3 + 8k^2 + 4k}{3} = \frac{(k^2 + 2k + 1)(k^2 + 2k + 1) + (k^2 + 2k + 1)(k+1) - k^2 - 2k - 1 - k - 1}{3}$$

$$\frac{k^4 + 5k^3 + 8k^7 + 4k}{3} = \frac{k^4 + 5k^3 + 8k^7 + 4k}{3}.$$

We have proved that the LHS equals to the RHS, thus the proof of the lemma is finished. □

3.2.2 Sum of Combined Distances between Pairs of Center and Border Vertices

Lemma 3.10. Let k bcc unit cells be connected in a row and another new bcc cell is connected to the end of this row. Then the sum of combined distances between old centers and new border vertices plus the sum of combined distances between the new center and old border vertices is

$$\frac{32k^3+120k^2+136k+48}{3}. \tag{3.12}$$

Proof: Observe on Figure 4 (on the right) how the 4 new border vertices are connected to the new center and old centers, and the old border vertices are connected to the new center. The sum of these distances can be written in the following form (see also the proof of Lemma 3.4).

$$\underbrace{(4\cdot 1)+(4\cdot 3)+(4\cdot 5)+(4\cdot 7)+...+4(2k+1)}_{(new\ border\ vertices\ to\ all\ centers)}+\underbrace{(4\cdot 1)+(4\cdot 3)+(4\cdot 5)+(4\cdot 7)+...+4(2k+1)}_{(old\ border\ vertices\ to\ new\ center)}=$$

$$=2(4\cdot 1+4\cdot 3+4\cdot 5+4\cdot 7+...+4(2k+1))=8(1+3+5+7+...+(2k+1))=8(k+1)^2.$$

The second moment part of the combined distances is given by the sum of the squares of the same values:

$$=2(4\cdot(1)^2+4\cdot(3)^2+4\cdot(5)^2+4\cdot(7)^2+...+4(2k+1)^2)=8((1)^2+(3)^2+(5)^2+(7)^2+...+(2k+1)^2)=$$

$$\frac{8((k+1)(2k+1)(2k+3))}{3}=\frac{32k^3+96k^2+88k+24}{3}.$$

By adding two equations, we have:

$$8(k+1)^2+\frac{32k^3+96k^2+88k+24}{3}=$$

$$\frac{24k^2+48k+24}{3}+\frac{32k^3+96k^2+88k+24}{3}=\frac{32k^3+120k^2+136k+48}{3}.$$

Thus the proof of the lemma is finished. □

Lemma 3.11. Let n bcc unit cells be connected in a row. Then the sum of combined distances between center vertices and border vertices in this bcc grid graph is given by

$$\frac{8n^4 + 24n^3 + 16n^2}{3}. \tag{3.13}$$

Proof: The proof goes by induction.

The base of the induction is the case $n = 1$. In this case, there is only 1 center, and it is connected to every of the 8 corners (border points) of the unit cell having unit distances. The sum of these distances and their squares is 16, and also, formula (3.13) gives this value. Now let us assume that the formula holds up to a value k. Let us prove that it also holds for the value k+1. By Lemma 3.10, we know the combined distance obtained by the centers (old and new) and border vertices (old and new). Applying this, with the induction hypothesis gives the following statement that is needed to be proven:

$$\frac{8k^4 + 24k^3 + 16k^2}{3} + \frac{32k^3 + 120k^2 + 136k + 48}{3} = \frac{8(k+1)^4 + 24(k+1)^3 + 16(k+1)^2}{3}.$$

After mathematical simplification, we have the following:

$$\frac{8k^4 + 56k^3 + 136k^2 + 136k + 48}{3} = \frac{8k^4 + 56k^3 + 136k^2 + 136k + 48}{3}.$$

Now, we proved that LHS equals to the RHS.

Thus the proof of the lemma is finished. □

3.2.3 Sum of Distances between Pairs of Border Vertices

Lemma 3.12. Let k bcc unit cells be connected in a row. If a new bcc 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 border vertices is

$$\frac{64k^3+336k^2+560k+396}{3}. \tag{3.14}$$

Proof: First of all, the sum of distances between any pair of the 4 new vertices is 12. (See the proof of Lemma 3.6).

Now, let us take the distance between one of the new border vertices (e.g., v_{N_1}) and all old border vertices:

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

We multiply it by 4 since we have 4 new vertices (v_{N_1}, v_{N_2}, v_{N_3}, v_{N_4}). Thus we have:

$$16(k+1)(k+2)\ .$$

Finally, the total sum of distances between all new and old border vertices is given by the sum of the previous two values is:

$$16(k+1)(k+2)+12\ .$$

Now, we have to compute the sum of the square of the distances. First of all, the total sum of the square of the distance between each pair of new border vertices is $6{\cdot}2^2 = 24$. Next, we have

$$16(2^2+4^2+6^2+...+2(k+1)^2)=\frac{16(2k+1)(k+2)(2k+3)}{3}=\frac{64k^3+288k^2+416k+192}{3}$$

Finally, the total sum is:

$$\frac{64k^3+288k^2+416k+192}{3}+24+16(k+1)(k+2)+12=\frac{64k^3+336k^2+560k+396}{3}.$$

Thus, the proof is finished. □

Lemma 3.13. Let n bcc unit cells be connected in a row. Then the sum of combined distances between pairs of border vertices is given by

$$\frac{16n^4+80n^3+128n^2+172n+108}{3}. \tag{3.15}$$

Proof: The proof goes by induction.

The base of the induction is the case $n = 1$. In this case, there is only 1 center, and it is connected to every of the 8 corners (border points) of the unit cell having unit distances. The sum of combined distances between all pairs of border vertices is 168, and also, formula (3.15) gives this value. Now, let us assume that the formula holds up to a value k. Let us prove that it also holds for the value k+1. By Lemma 3.12, we know the combined distances obtained by the old and new border vertices. Applying this, with the induction hypothesis gives the statement that is needed to be proven. In this proof, we have to prove that the LHS equals to the RHS.

$$\frac{16k^4+80k^3+128k^2+172k+108}{3}+\frac{64k^3+336k^2+560k+396}{3}=$$
$$=\frac{16(k+1)^4+80(k+1)^3+128(k+1)^2+172(k+1)+108}{3}.$$

The simplification process for the RHS is:

$$\frac{16(k^4+4k^3+6k^2+4k+1)+80(k^3+3k^2+3k+1)+128(k^2+2k+1)+172k+172+108}{3}$$

$$\frac{16k^4+64k^3+96k^2+64k+16+80k^3+240k^2+240k+80+128k^2+256k+128+172k+172+108}{3}$$

The result can be proven based on basic mathematical simplifications/modifications to prove that the LHS equals to the RHS:

$$\frac{16k^4+144k^3+464k^2+732k+504}{3}=\frac{16k^4+144k^3+464k^2+732k+504}{3}.$$

The proof of the lemma is finished. □

3.2.4 Formula for hyper-Wiener Index

Based on the previous lemmas, we are ready to state our second main result.

Theorem 3.2: Let n be the number of bcc unit cells that are connected in a row. Then the formula to find WW for grid of bcc unit cells connected in row,

$$WW(G)=\frac{25n^4+105n^3+143n^2+171n+108}{6}. \tag{3.16}$$

Proof: The final formula to calculate WW, see equation (3.9), is, actually, the sum of equations (3.11), (3.13) and (3.15). All possible distances are considered in exactly once in the Lemmas 3.9, 3.11 and 3.13, and then, by simple calculation the sum of those formulas

$$\frac{1}{2}\left(\frac{n^4+n^3-n^2-n}{3}+\frac{8n^4+24n^3+16n^2}{3}+\frac{16n^4+80n^3+128n^2+172n+108}{3}\right)$$

$$=\frac{25n^4+105n^3+143n^2+171n+108}{6}.$$ □

So we have general formula to find hyper-Wiener index WW for bcc unit cells that are connected in a row.

3.3 Connection to Integer Sequences

In order to have the ability to compute WI and WW for bcc grid graphs, three different subsums are used in both cases. In this section we show some interesting connections between the subsums presented in equations (3.3), (3.5) and (3.7) and well-known sequences given in the famous library of integer sequences by Sloane [29].

Equation (3.7), the subsum for border vertices, $\frac{16(n+1)^3+20(n+1)}{3}$ is identified in [29], as A001386. In [24] this sequence is described as a coordination sequence (giving the number of vertices that are located from a given distance from a chosen vertex of a lattice/grid) for 4-dimensional I-centered tetragonal orthogonal lattice (to obtain our sequence the first two elements of A001386 should be deleted).

The sequence defined by equation (3.3), $\frac{n^3-n}{3}$ can also be found in Sloane's. It is A007290 and the values are, actually, the doubles of values of the binomials $\binom{n}{3}$. This sequence appear in various places in physics, mathematics, and specially, in graph theory, as well. Moreover, this sequence also gives the reverse *WI* of the path graph with *n* vertices [3].

The integer sequences defined by equation (3.5), (3.8), (3.11), (3.13), (3.15) and (3.16) are not found in [29].

Table 1 shows some of the first elements of the sequences we are working with, i.e., the values computed by equations (3.3), (3.5), (3.7), (3.8), (3.11), (3.13), (3.15) and (3.16) for some small values of *n*. The *WI* and *WW* values are shown in the table.

Table 1: Some values of the subsums and *WI* and *WW* for few bcc unit cells in a row.

Number of bcc unit cells (n)	1	2	3	4	5	6	7
Equation (3.3)	0	2	8	20	40	70	112
Equation (3.5)	8	40	112	240	440	728	1120
Equation (3.7)	56	164	368	700	1192	1876	2784
Wiener index *WI*	**64**	**206**	**488**	**960**	**1672**	**2674**	**4016**
Equation (3.11)	0	6	32	100	240	490	896
Equation (3.13)	16	128	480	1280	2800	5376	9408
Equation (3.15)	168	620	1744	4020	8056	14588	24480
Hyper-Wiener index *WW*	**92**	**377**	**1128**	**2700**	**5548**	**10277**	**17392**

Chapter 4

WIENER INDEX AND HYPER-WIENER INDEX ON ROWS OF UNIT CELLS OF THE FACE-CENTERED CUBIC LATTICE

4.1 Wiener Index for a Row of fcc Unit Cells

In this section we present our results about *WI* in the fcc grid. In the next subsections some subsums are computed that are needed later on. We start from a straightforward result:

Lemma 4.1. Let n be the number of fcc unit cells connected in a row, the number of all vertices $|V|_{all}$ (border points and central points) in this graph is given by

$$|V|_{all} = (9n+5). \tag{4.1}$$

The number of border points $|V_b|$ for n fcc unit cells connected in a row is calculated using the formula

$$|V_b| = (4n+4). \tag{4.2}$$

The number of central points $|V_c|$ row is calculated using the formula

$$|V_c| = (5n+1). \tag{4.3}$$

4.1.1 Sum of Distances between Central Points

In our work, we will use the following terminology for central points: we differentiate side center points and shared center points. By side centers we mean the centers that are located in the center of each face of a unit cell that is not being shared when we add a new unit cells to the end of the row (e.g., C_2, C_5 in Figure 5).

Shared centers are the center points that are common and shared between two fcc unit cells connected in a row (e.g., C_3 in Figure 5).

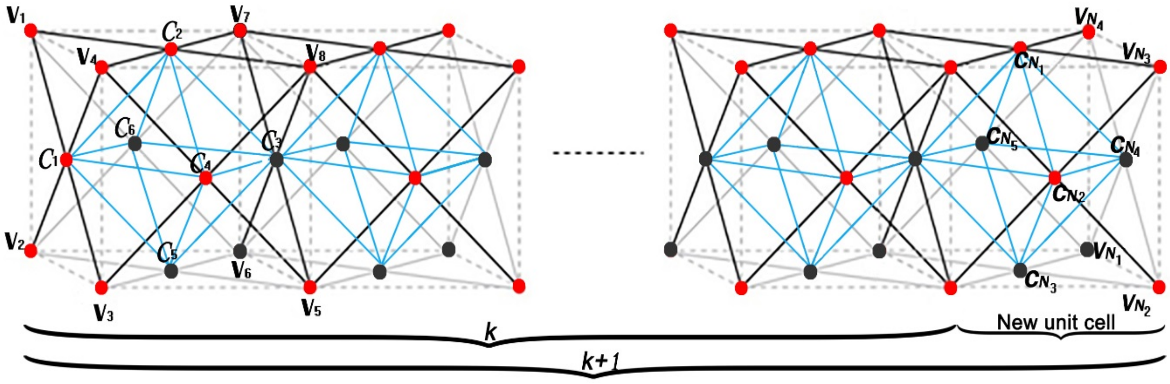


Figure 5: k fcc unit cells connected in a row with a new unit cell attached the end of the row

Lemma 4.2. Let k fcc unit cells be connected in a row. 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 all distances between the pairs of new central points (shared and side central points) and between new central points and old central points (shared and side central points) is

$$25k^2 + 35k + 18\,. \tag{4.4}$$

Proof:

In our proof, we will calculate the sum of total distance as follows:

- First of all, and according to Figure 5, the sum of total distance between the pairs built up from the new five center points equals to

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

- Next, we will calculate the distance between the new shared center (C_{N_4}) and old shared centers (including C_1). We have

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

- Next, we will calculate the distance between new side centers and old shared centers. So we have $1+3+5+\cdots+(2k+1)=(k+1)^2$. Then we multiply it by 4 since we have 4 new side centers to get the formula $4(k+1)^2$.

- Next, we need to calculate the distance between new side centers i.e., $C_{N_1}, C_{N_2}, C_{N_3}, C_{N_5}$ and old side centers. For any of the new side centers we have

$$(2\cdot 4)+(4\cdot 4)+\cdots+(2k\cdot 4)=8+16+24+32+\cdots+8k=$$
$$8(1+2+3+4+\cdots+k)=8\left(\sum_{i=1}^{k} i\right)=8\frac{k(k+1)}{2}+1=4k^2+4k.$$

  Then we multiply it by 4 since we have 4 new side centers to get the formula $16k^2+16k.$

- Finally, we will calculate the distance between the new shared center, i.e., C_{N_4} and all old side centers: $4(3+5+7+\cdots+(2k+1))=4((k+1)^2-1)$ the formula is given by $4k^2+8k$.

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:

$$12+k^2+3k+2+4(k+1)^2+16k^2+16k+4k^2+8k=25k^2+35k+18. \qquad \square$$

Lemma 4.3. Let *n* fcc unit cells be connected in a row. Then the sum of all distances between central points (side and shared points) in this (segment of the) fcc grid graph is given by

$$\frac{25n^3+15n^2+14n}{3}. \tag{4.5}$$

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 centers (side and shared center points), and the sum of distances between these central points equals to 18 (there are 12 pairs of neighbour centers and 3 pairs such that they are opposite to each other, and thus, their distance is 2), and the formula (4.5) 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 4.2, we know the sum of the distances obtained by the new central points and old centrals. Applying this, with the induction hypothesis, we must prove that the LHS equals to the RHS, so we have:

$$\frac{25k^3+15k^2+14k}{3}+(25k^2+35k+18)=\frac{25(k+1)^3+15(k+1)^2+14(k+1)}{3}.$$

$$\frac{25k^3+15k^2+14k}{3}+\frac{75k^2+105k+54}{3}=\frac{25(k+1)^3+15(k+1)^2+14(k+1)}{3}$$

$$\frac{25k^3+90k^2+119k+54}{3}=\frac{25k^3+75k^2+75k+25+15k^2+30k+14k+29}{3}$$

$$\frac{25k^3+90k^2+119k+54}{3}=\frac{25k^3+90k^2+119k+54}{3}.$$

So the LHS equals to the RHS and the proof of the induction is complete. By the induction, it follows that formula (4.5) is true for all (non-negative integer value of) n. □

4.1.2 Sum of distances between Central Points and Border Points

In these subsections we compute the distances between (side and shared) central points and border points.

Lemma 4.4. Let k fcc unit cells be connected in a row and let a new fcc unit cell be connected to the end of this row. Then the sum of the distances between old central points and new border points plus the sum of the distances between the new central points and old border points is

$$40k^2 + 88k + 68. \tag{4.6}$$

Proof:

In this proof we have to calculate the sum of total distance in the following ways:

- The sum of the distance between one of the new border points (e.g. v_{N_1}) and all shared centers, we have

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

  We have to multiply it by 4 since we have 4 new border points and the formula is

  $$4k^2+12k+8.$$

  - The sum of the distance between one of new border points and all side centers: $4(3+5+7+\cdots+(2k+1)) = 4((k+1)^2-1) = 4k^2+8k$;

  It needs to be multiplied by 4, since we have 4 new border points: the formula for this sum will be

  $$16k^2+32k.$$

- The total sum of the distances between new border points and new side centers is 24. The total sum of the distances between new border points and new shared centers (i.e., C_{N_4}) is $\sum_{i=1}^{4}(V_{N_i}, C_{N_4}) = 4$. The total sum of new border points and new centers is $\sum_{i=1}^{4}\sum_{j=1}^{5} d_G(V_{N_i}, C_{N_j}) = 28$. (For each of the four border points it is $3\cdot 1 + 2\cdot 2$)

- The sum of distances between old border points and the new shared center (C_{N_4}) is:

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

- The sum of the distance between old border points and new side center points is given by

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

Finally, the final formula to calculate the total sum of the distances between old central points and new borders points plus the sum of the distances between the new central points and old border points plus the sum of distances between new border and center points is the sum of all previous distances, i.e.,:

$$4k^2+12k+8+16k^2+32k+24+4+4k^2+12k+8+16k^2+32k+24 = 40k^2+88k+68.$$ □

Lemma 4.5. Let n fcc unit cells be connected in a row. Then the sum of all distances between central points and border points in this fcc grid graph is given by

$$\frac{40n^3+72n^2+92n+12}{3}. \tag{4.7}$$

Proof: The proof goes by induction on n.

The base of the induction is the case $n = 1$. In this case, there is only 6 centers, and it is connected to every of the 8 corners (border points) of the unit cell as follows: Each center has 4 neighbour border points and 4 other border points with distance 2. In this way, the sum is $(4+4\cdot 2)\cdot 6 = 72,$ and also, formula (4.7) 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 4.4, we know the sum of the new distances obtained between old central points and new border points (of the $(k + 1)$st unit cell), between the centers 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 gives the following statement that is needed to be proven:

We have to prove that the LHS equals to the RHS:

$$\frac{40k^3+72k^2+92k+12}{3}+(40k^2+88k+68)=\frac{40(k+1)^3+72(k+1)^2+92(k+1)+12}{3}$$

$$\frac{40k^3+72k^2+92k+12}{3}+\frac{(120k^2+264k+204)}{3}=\frac{40(k+1)^3+72(k+1)^2+92(k+1)+12}{3}$$

$$\frac{40k^3+192k^2+356k+216}{3}=\frac{40k^3+120k^2+120k+40+72k^2+236k+176}{3}$$

$$\frac{40k^3+192k^2+356k+216}{3}=\frac{40k^3+192k^2+356k+216}{3}.$$

Now, we proved that the LHS equals to the RHS. □

4.1.3 Sum of Distances of Border Points

Lemma 4.6. 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 all distances between new and old border points is

$$16k^2+48k+48. \tag{4.8}$$

Proof: Observe that the sum of distances between all pairs of the 4 new vertices is 12. (See Figure 5, 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).

Now, let us compute the sum of distances between one of the new border points (e.g., v_{N_1}) and all old border 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 border vertices (v_{N_1}, v_{N_2}, v_{N_3}, v_{N_4}).

Thus we have:

$$4(4(k+1)(k+2)+1)=16(k+1)(k+2)+4$$

Finally, the total sum of distances between all new and old border points is given by the sum of the previous two values:

$$16(k+1)(k+2)+4+12=16k^2+48k+48.$$

Thus, formula (4.8) is obtained. □

Lemma 4.7. Let *n* fcc unit cells be connected in a row. Then the sum of all distances between pairs of border points is given by

$$\frac{16n^3+48n^2+80n+36}{3}. \tag{4.9}$$

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 (border points) of the unit cell. Each pair of them has a distance 2, but pairs of opposite corners that have distance 3, therefore the sum of distances between all pairs of border vertices is: $24\cdot 2+4\cdot 3=60.$ As one can easily check, formula (4.9) gives the same 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 4.6, we know the sum of the distances obtained by the old and new border points. Applying this, with the induction hypothesis gives the statement that is needed to be proven

$$\frac{16k^3+48k^2+80k+36}{3}+(16k^2+48k+48)=\frac{16(k+1)^3+48(k+1)^2+80(k+1)+36}{3}$$

$$\frac{16k^3+48k^2+80k+36}{3}+\frac{(48k^2+144k+144)}{3}=\frac{16(k+1)^3+48(k+1)^2+80(k+1)+36}{3}$$

$$\frac{16k^3+96k^2+224k+180}{3}=\frac{16(k+1)^2(k+1)+48(k^2+2k+1)+80k+80+36}{3}$$

$$\frac{16k^3+96k^2+224k+180}{3}=\frac{16k^3+96k^2+224k+180}{3}.$$

So the LHS equals to the RHS. □

4.1.4 Sum of All Distances: The Main Formula

Based on the results proven in the previous three subsections, we are able to state our first main result about fcc grid graph.

Theorem 4.1. Let n be the number of fcc unit cells that are connected in a row. Then the formula to find WI for this graph is:

$$WI(n)=27n^3+45n^2+62n+16. \tag{4.10}$$

Proof: The formula is the sum of equations (4.5), (4.7) and (4.9). All possible distances are considered in exactly one of the Lemmas 4.3, 4.5 and 4.7, and then, we will prove it using direct proof by finding the sum of equations (4.5), (4.7) and (4.9). So we have

$$\frac{25n^3+15n^2+14n}{3}+\frac{40n^3+72n^2+92n+12}{3}+\frac{16n^3+48n^2+80n+36}{3}$$, and thus,

$$WI(n)=27n^3+45n^2+62n+16.$$

Our theorem, the formula of equation (4.10), is proven. □

Using formula (4.10) one can calculate WI for graph of fcc unit cells connected in a row, as we will present some examples in the next table.

Table 2. Shows some of the first elements of the sequences we are working with, i.e., the values computed by equations (4.5), (4.7), (4.9) and (4.10) for some small values of n. The *WI* values are shown in the last row of the table.

Table 2: Some values of the subsums and *WI* for few fcc unit cells in a row

Number of fcc unit cells in a row (n)	1	2	3	4	5	6
Equation (4.9)	60	172	380	716	1212	1900
Equation (4.7)	72	268	672	1364	2424	3932
Equation (4.5)	18	96	284	632	1190	2008
Wiener index *WI*	**150**	**536**	**1336**	**2712**	**4826**	**7840**

4.2 Computing the hyper-Wiener Index for fcc Unit Cells connected in a Row

The general formula to compute *WW* for a graph is given in (4.11):

$$WW(G) = \frac{1}{4} \sum_{u,v \in V(G)} \left(d_G(u,v) + d_G^2(u,v) \right), \tag{4.11}$$

We are computing *WW* again by summing up combined distance as we did in section 3.2 and 3.2.4 for bcc grid. In fcc grid we have to compute the distance between:

- unordered pairs of face centers,
- pairs of face centers 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 same formula works for a graph containing k+1 unit cells in a row. In proofs we refer to Figure 5.

To make our computation more readable and more easily understandable we differentiate two subtypes of face centers:

- the side centers (or side center 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 5; and
- the shared centers (or shared center points) are the face centers on the squares, either on the two ends or somewhere inside the body, e.g., C_1 and C_3 in Figure 5.

4.2.1 Sum of combined Distances between Pairs of Face Centers

Let us start by computing how much the sum of combined distances among face centers increases when a new unit cell is attached to the end of the row (Figure 5).

Lemma 4.8. 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 centers and between pairs of a new and an old face center is

$$\frac{100k^3 + 285k^2 + 251k + 126}{3} \tag{4.12}$$

Proof:

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

- First of all, and according to Figure 5, the sum of distances between the pairs built up from the new five center 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 center C_{N_4} is 1 from the new side centers, e.g. C_{N_1}; there are 4 pairs of neighbour side centers, e.g., C_{N_1} and C_{N_2}; and finally, there are 2 pairs of non-neighbour side centers, 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 center points equals to 16. This is summed up as 12 + 16 = 28.

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

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

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

The sum of their squares,

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

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

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 centers and old shared centers. So we have $1+3+5+\cdots+(2k+1)=(k+1)^2$. Then we multiply it by 4 since we have 4 new side centers to get the formula $4(k+1)^2$.

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 centers i.e., C_{N_1}, C_{N_2}, C_{N_3} C_{N_5} and old side centers. For any of the new side centers we have

$$(2 \cdot 4) + (4 \cdot 4) + \cdots + (2k \cdot 4) = 8 + 16 + 24 + 32 + \cdots + 8k =$$
$$8(1 + 2 + 3 + 4 + \cdots + k) = 8\left(\sum_{i=1}^{k} i\right) = 8\frac{k(k+1)}{2} + 1 = 4k^2 + 4k.$$

Then we multiply it by 4 since we have 4 new side centers 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 formulas:

$$\frac{64k^3 + 96k^2 + 32k}{3} + 16k^2 + 16k = \frac{64k^3 + 144k^2 + 80k}{3}.$$

- Finally, we will calculate the sum of the distances between the new shared center, i.e., C_{N_4} and all old side centers:

$$4(3+5+7+\cdots+(2k+1)) = 4((k+1)^2 - 1),$$

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 4.9. Let n fcc unit cells be connected in a row. Then the sum of combined distances between center vertices in this fcc grid graph is

$$\frac{25n^4+45n^3+8n^2+48n}{3}. \tag{4.13}$$

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 centers (both side and shared center points are counted), and the sum of combined distances between these central points equals to 42 (there are 12 pairs of neighbour centers and 3 pairs such that they are opposite to each other, and thus, their distance is 2), and the formula (4.13) 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 4.8, 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 LHS equals to the RHS, 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 LHS equals to the RHS and the proof of the induction is complete. By the induction, it follows that formula (4.13) is true for all (non-negative integer value of) n. □

4.2.2 Sum of combined Distances between pairs of Face Centers and Cube Vertices

Lemma 4.10. Let k fcc unit cells be connected in a row and another, new, fcc unit cell is connected to the end of this row. Then the sum of combined distances between old face centers and new cube vertices plus the sum of combined distances between pairs formed by a new face center and an old cube vertex is

$$\frac{160k^3+648k^2+824k+552}{3}. \tag{4.14}$$

Proof: In this proof we have to calculate the sum of total distance in the following ways:

- The sum of the distance between one of the new border points (e.g. v_{N_1}) and all old shared centers, we have

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

  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

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

  The sum of two previous formulas are:

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

- The sum of the distance between one of the new cube points and all side centers is**:**

$$4(3+5+7+\cdots+(2k+1))=4((k+1)^2-1)=4k^2+8k\ ;$$

It needs to be multiplied it by 4, since we have 4 new border points: the formula for this sum will be

$$16k^2+32k.$$

The sum of the second moment is:

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

By summing up the two formulas, 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 centers is 24 (8 times 1, when the cube vertex is of the corner of the same square as the face center 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 centers is $8\cdot1^2+8\cdot2^2=40$. Further, the total sum of the distances between new cube vertices and the new shared center (i.e., C_{N_4}) is $\sum_{i=1}^{4}(V_{Ni},C_{N4})=4$ (all the 4 new cube points are neighbours of the new shared center). Moreover, the sum of the squares of the distances between the new cube points and the new shared center is also 4. (The total sum of distances between new cube points and new face centers 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 $(3\cdot1+2\cdot2)$. 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 center, C_{N_4}, is

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

The sum of the squares is:

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

The sum of two previous formulas are:

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

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

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

The sum of the squared distance is:

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

The sum of two previous formulas are:

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

Finally, the formula to calculate the total sum of the combined distances between old face center points and new cube points, plus the sum of the combined distances between the new face center points and old cube points, plus the sum of combined distances between new cube points and new face centers, 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 4.11. Let n fcc unit cells be connected in a row. Then the sum of combined distances between center vertices and border vertices in this fcc grid graph is given by

$$\frac{40n^4+136n^3+128n^2+248n+24}{3}. \tag{4.15}$$

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 centers, and 8 cube points. Each face center has 4 neighbour cube vertices, and 4 other at distance 2. In this way, the combined distance between face centers and cube vertices is $6(4+4\cdot2+4\cdot1^2+4\cdot2^2) = 192$ and also, formula (4.15) 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 4.10, 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 centers 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, we have to prove that the LHS equals to the RHS:

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

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

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

Now, we proved that the LHS equals to the RHS. □

4.2.3 Sum of Combined Distances between Pairs of Cube Vertices

Lemma 4.12. 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

$$\frac{64k^3+336k^2+560k+468}{3}. \tag{4.16}$$

Proof: In this proof we have to calculate the sum of total distance in the following ways:

- Observe that the sum of distances between all pairs of the 4 new cube vertices is summed up to 12. (See Figure 5, 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 distance between each pair 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 it by 4 since we have 4 new cube vertices (V_{N_1}, V_{N_2}, V_{N_3}, and V_{N_4}). Thus, the sum of distances is

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

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

$$\begin{aligned}
&4(2^2\cdot 4+4^2\cdot 4+6^2\cdot 4+\cdots+(2(k+1))^2\cdot 4)+4\cdot 3^2-4\cdot 2^2 = \\
&16\cdot 4(1^2+2^2+3^2+\cdots+(k+1)^2)+20=\frac{16(2k+2)(k+2)(2k+3)}{3}+20 \\
&=\frac{64k^3+288k^2+416k+192}{3}+20=\frac{64k^3+288k^2+416k+252}{3}
\end{aligned}$$

$$\frac{64k^3+288k^2+416k+192}{3}+\frac{60}{3}=\frac{64k^3+288k^2+416k+525}{3}$$

Finally, the total combined sum is:

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

Thus, formula (4.16) is obtained. □

Lemma 4.13. Let *n* fcc unit cells be connected in a row. Then the sum of combined distances between pairs of cube vertices is given by

$$\frac{16n^4+80n^3+128n^2+244n+108}{3}. \tag{4.17}$$

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 (4.17) 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 4.12, we know the sum of the combined distances obtained by the old and new border points. Applying this, with the induction hypothesis gives the statement that is needed to be proven

$$\frac{16k^4 + 80k^3 + 128k^2 + 244k + 108}{3} + \frac{64k^3 + 336k^2 + 560k + 468}{3} =$$
$$= \frac{16(k+1)^4 + 80(k+1)^3 + 128(k+1)^2 + 244(k+1) + 108}{3}$$

For the right hand part, we have the following mathematical simplifications:

$$= \frac{16(k^4 + 4k^3 + 6k^2 + 4k + 1) + 80(k^3 + 3k^2 + 3k + 1) + 128(k^2 + 2k + 1) + 244k + 244 + 108}{3}$$

$$\frac{16k^4 + 64k^3 + 96k^2 + 64k + 16 + 80k^3 + 240k^2 + 240k + 80 + 128k^2 + 256k + 128 + 244k + 244 + 108}{3}$$
$$\frac{16k^4 + 144k^3 + 464k^2 + 804k + 576}{3}$$

After that we have

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

Thus, the LHS equals to the RHS. □

4.2.4 The Hyper-Wiener Index

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

Theorem 4.2: Let n be the number of fcc unit cells that are connected in a row. Then the formula to find WW for grid of fcc unit cells connected in row,

$$\frac{81n^4 + 261n^3 + 264n^2 + 540n + 132}{6}. \tag{4.18}$$

Proof:

The final formula to calculate *WW* (see eq. 3.9) is the half sum of equations (4.13), (4.15) and (4.17). All possible distances are considered in exactly one of the lemmas 4.9, 4.11 and 4.13, and then, by simple calculation the sum of those formulas

$$\frac{1}{2}\left(\frac{25n^4+45n^3+8n^2+48n}{3}+\frac{40n^4+136n^3+128n^2+248n+24}{3}+\frac{16n^4+80n^3+128n^2+244n+108}{3}\right)$$

$$=\frac{1}{2}\left(\frac{81n^4+261n^3+264n^2+540n+132}{3}.\right)$$

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

So we have the general formula to find *WW* for graphs of fcc unit cells that are connected in a row.

Table 3 shows some of first elements of our sequences, i.e., the values computed by equations (4.13), (4.15), (4.17) and (4.18) for some small value of *n*.

Table 3: Some values of the subsums, and *WW* for few fcc unit cells in a row.

Number of fcc unit cells (n)	1	2	3	4	5
Equation (4.13)	42	296	1152	3200	7230
Equation (4.15)	192	920	2944	7336	15488
Equation (4.17)	192	668	1816	4116	8176
Hyper-Wiener index *WW*	213	942	2956	7326	15477

Chapter 5

CONCLUSION AND FUTURE WORK

5.1 Conclusions

Grids, and specially, non-traditional three-dimensional grids are lying in the intersection of digital and discrete geometry, graph and lattice theory, crystallography and other applied fields in physics and chemistry. One of the most important topological/geometrical indices of graph structure is the *WI*. *WI* is a graph invariant that belongs to the molecular structure descriptors, called topological indices. These indices are widely used by chemists to design molecules with desired properties. After the success of *WI*, several other important topological/geometrical indices are defined for various graph structures; one of those is the *WW*. *WW* is also used as a structure-descriptor for detecting physicochemical characteristics of organic compounds. It is one of the recent distance-based graph invariants, often used for agriculture, pharmacology, environment-protection, etc.

In this thesis, the bcc grid is investigated in which a finite number of unit cells are placed next to each other at a line. We have formulated and proved the computation of *WI* and *WW* for these graphs. The fcc lattice is analysed also in this thesis, especially, when a finite number of unit cells are placed next to each other at a line. We have presented and proved formulas for the computation of *WI* and *WW* for fcc grid graphs.

5.2 Future Work

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 index for these graphs. The Szeged index of a graph G is computed as follows: for each edge $e_{u,v}$ of the graph G, let $n_u(e)$ be the number of vertices w of G that has smaller distance $d_G(u,w)$ from vertex u than from vertex v. Then the sum $\sum_{e_{u,v}\in E(G)} n_u(e)n_v(e)$ gives the Szeged index of G. See, for instance, [19], for some calculations of Szeged index of some two-dimensional regular grid graphs.
- One can extend the results to two and three dimensional rectangles and blocks of unit cells both for fcc grids and bcc grids.
- Moreover, other non-traditional grids, e.g., $n\times 1\times 1$ diamond cubic grid can also be involved to similar studies.
- Moreover, other non-traditional grids, e.g., $n\times n\times 1$ fcc grid can also be involved to similar studies.
- 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 these indices are related to some of these properties and thus these indices can have direct applications.

REFERENCES

[1] Al-Kandari, A., Manuel, P., & Rajasingh, I. (2011).Wiener index of Sodium Chloride and Benzenoid Structures. *The Journal of Combinatorial Mathematics and Combinatorial Computing*, 79, 33–42.

[2] Balaban, A. T., Mills, D., Ivanciuc, O., & Basak, S. C. (2000). Reverse Wiener indices, *Croatica Chemica Acta*, 73, 923-941.

[3] Baskar B. J., & Ramakrishnan, S. (2012). Topological Indices and New Graph Structures. *Applied Mathematical Sciences*, 6(108), 5383 – 5401.

[4] Bollobás, B. (1979). *Graph theory: An Introductory Course*, Springer-Verlag, New York.

[5] Cash, G., Klavzar, S., & Petkovsek, M. (2002). Three Methods for Calculation of the hyper-Wiener index of Molecular Graphs. *J. Chem. Inf. Comput. Sci*., 42, 571-576.

[6] Cerruela, G., Luque R. I., Gómez-Nieto M. A., Cabrero Doncel, J.A., & Guevara Plaza, A. (2005). From Wiener index to molecules. *J. Chem. Inf. Model.* 45(2), 231-238.

[7] Chepoi, V., & Klavžar, S. (1997). The Wiener index and the Szeged index of Benzenoid Systems in Linear Time, *J. Chem. Inf. Comput. Sci*., 37*,* 752-755.

[8] Daneshvar, S., Izbirak, G., & Kaleibar, M. (2012). Topological Indices of Hypercubes, *Journal of Basic and Applied Scientific Research*, 2(11), 11501-11505.

[9] Dobrynin, A. A., Gutman, I., Klavžar, S., & Žigert, P. (2002).Wiener index of hexagonal systems. *Acta Appl. Math.,* 72, 247–294.

[10] Graovac, A., & Pisanski, T., (1991). On the Wiener index of a graph, *Journal of Mathematical Chemistry*, 8(1), 53-62.

[11] Harishchandra S. R., Deepak S. R., & Asha B. G. (2012). On The Wiener index of Agraph, *J. Indones. Math. Soc*., 18(1), 57-66.

[12] Heydari, A., & Gutman. I. (2010). On The Terminal Wiener index of Thorn Graphs. *Kragujevac J. Sci*., 32, 57-64.

[13] John, P. E., & Diudea M. V. (2004). Wiener index of zig-zag polyhex nanotubes, *Croatica Chemica Acta,* 77**,** 127-132.

[14] Khalifeh, M. H., Yousefi-Azari, H., & Ashrafi, A.R. (2008). The hyper-Wiener index of graph operations, *Computers and Mathematics with Applications*, 56, 1402–1407.

[15] Kittel, C. (2004). *Introduction to Solid State Physics*, Wiley, New York.

[16] Klavžar, S., Zigerta, P., & Gutman. I. (2000). An algorithm for the calculation of the hyper-Wiener index of benzenoid hydrocarbons. *Computers and Chemistry*, 24, 229 – 233.

[17] Klein, D. J., Lukovits I., & Gutman I. (1995). On the definition of the hyper-Wiener index for cycle-containing structures. *J. Chem. Inf. Comput. Sci.,* 35, 50-52.

[18] Klette, R., & Rosenfeld, A. (2004). *Digital geometry – geometric methods for digital picture analysis*. Morgan Kaufmann.

[19] Manuel, P., Rajasingh, I., & Arockiaraj, M. (2012). Wiener and Szeged indices of Regular Tessellations, ICINT 2012, IPCSIT, 37, 210–214.

[20] Mohar, B., & Pisanski, T. (1988). How to compute the Wiener index of a graph. *J. Math. Chem.*, 2, 267–277.

[21] Mujahed, H., & Nagy, B. (2015).Wiener index on Lines of Unit Cells of the body-centered cubic Grid. ISMM 2015: 12th International Symposium on Mathematical Morphology and Its Applications to Signal and Image Processing, *LNCS* 9082, 597–606.

[22] Mujahed, H., & Nagy, B. (2016). Wiener index on rows of unit cells of the face-centred cubic lattice. *Acta Cryst.* A72, 243-249.

[23] Nagy, B., & Strand, R. (2008). Non-Traditional Grids Embedded in Z^n. *International Journal of Shape Modeling*, 14, 209–228.

[24] O'Keeffe, M. (1995). Coordination sequences for lattices, *Zeit. f. Krist*., 210, 905-908.

[25] Plavšić, D., Nikolić, S., Trinajstić, N., & Mihalić, Z. (1993). On the Harary index for the Characterization of Chemical Graphs. *J. Math. Chem.,* 12, 235-250.

[26] Randic, M. (1993). Novel molecular descriptor for structure-property studies, *Chemical Physics Letters*, 211, 478–483.

[27] Shigehalli, V. S., Misale, D. N., & Kuchabal, S. (2014). On the Hyper-Wiener index of graph Amalgamation, *Journal of Computer and Mathematical Sciences*, 5(4), 352-356.

[28] Shigehalli, V. S., & Kuchabal, S. (2014). On The hyper-Wiener index of Thorny-Complete Graph. *Journal of Global Research in Mathematical Archives*, 2(6).

[29] Sloane, N.: On-Line Encyclopedia of Integer Sequences (OEIS). (2014, May 2) Retrieved from http://oeis.org/

[30] Stephan G. Wagner, Hua Wang, & Gang Yu. (2009). Molecular graphs and the inverse Wiener index problem. *Discrete Applied Mathematics*, 157, 1544-1554.

[31] Strand, R., & Nagy, B. (2007). Distances based on neighborhood sequences in non-standard three-dimensional grids. *Discrete Applied Mathematics*, 155, 548–557.

[32] Strand, R., & Nagy, B. (2009). Path-based distance functions in *n*-dimensional generalizations of the face-and body-centered cubic grids. *Discrete Applied Mathematics*, 157, 3386–3400.

[33] Strand, R., Nagy, B., & Borgefors, G. (2011). Digital distance functions on three-dimensional grids. Theoretical Computer Science. 412, 1350–1363.

[34] Thilakam, K., & Sumathi, A. (2013). How to Compute the Wiener index of a Graph using Matlab, *International Journal of Applied Mathematics & Statistical Sciences*, 2(5), 143-148.

[35] Vijayabarathi, A., & Anjaneyulu, G.S.G.N. (2013). Wiener index of a graph and chemical applications, *International Journal of Chem. Tech. research*, 5(4), 1847-1853.

[36] Vukičević, D., & Trinajstić, N. (2004). Wiener Indices of Benzenoid Graphs. *Bulletin of the Chemists and Technologists of Macedonia*, 23(2), 113–129.

[37] Wiener, H. (1947). Structural determination of paraffin boiling points. *Journal of American Chemical Society*. 69, 17–20.

[38] Xing, R., Zhou, B., & Qi, X. (2011). Hyper–Wiener index of Unicyclic Graphs. *MATCH Commun. Math. Comput. Chem*., 66, 315–32.