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LECTURE ON TOPOLOGICAL CRYSTALLOGRAPHY

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Commemorating the fourth centennial anniversary of the publication of Kepler's pamphlet "New-Year's gift concerning six-cornered snow" (1611)

Abstract. This is an expository article on modern crystallography based on *discrete geometric analysis*, a hybrid field of several traditional disciplines: graph theory, geometry, theory of discrete groups, and probability, which has been developed in the last decade. The mathematical part relying on algebraic topology is fairly elementary, but may be still worthwhile for crystallographers who want to learn how mathematics is effectively used in the practical science. A brief history of crystallography is also explained.

1. Introduction

The main purpose of this expository article is twofold; first, to tell a brief history of crystallography, a practical science originated in the classification of the observed shapes of crystals, and second, to provide the reader with a mathematical insight into modern crystallography developed in the last two decades in order to bridge the gap of knowledge between mathematicians and crystallographers.

The mathematical tools employed here are adopted from elementary *algebraic topology*. More specifically, the routine theory of *covering spaces* and *homology groups* is effectively used in the study of the 3D networks associated with crystals. Actually many notions and tools invented by crystallographers may be interpreted in these algebraic-topological terms established by the first half of the 20th centuty (see Appendix). Moreover the enumeration of crystal structures, an area of considerable scientific interest for many years, is a simple byproduct of the classical theory of covering spaces as far as their topological structures are concerned (see Section 9 and 10).

In the latter part of the lecture, I shall explain a minimum principle for crystals in the framework of *discrete geometric analysis* ([39]), which characterizes *canonical placements*[1] of crystal structures, a way to place

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[1]This notion is the same as *standard realizations* introduced in [27], and coincides with the *archetypical representations* (Eon [23]); see Remark in Section 12).

them in space so as to have the most symmetric microscopic shapes. In its concrete construction, the well-known idea of orthogonal projections in *harmonic integrals* is employed. In spite of its pure-mathematical nature, the notion of canonical placements turns out to fit with a systematic design of crystal structures.

Canonical placements turn up in asymptotic behaviors of random walks on *topological crystals*, the abstraction of crystal structures, and are closely related to a discrete analogue of *Abel-Jacobi maps* in algebraic geometry as explained in Section 15. As a matter of fact, my initial motivation behind topological crystallography have arisen from these seemingly irrelevant subjects (see [28] and [30]).

This article is based on my lecture for the Summer Challenge project at High Energy Accelerator Research Organization (KEK) in Tsukuba. A full account of topological crystallography will be given in the forthcoming book [40]. See Eon [23] for an overview from crystallographer's standpoint.

Acknowledgement I am grateful to D. M. Proserpio and J.-G. Eon for fruitful discussions who also provided me with relevant references in chemical crystallography. I also thank Hisashi Naito and my daughter Kayo for producing the beautiful CG images of several hypothetical crystals.

2. Legacy of Ancient Greece in crystallography

Crystals, the word derived from the Greek meaning "ice", are the most stable form for all solids. They are found throughout the natural world, and have been always recognized as being distinct from other forms of matter.

The links between morphology of crystals and mathematics are ancient. It is said that geometry in ancient Greece started from the curiosity about the shapes of crystals[2]. Actually legend has it that Pythagoras (about 569 BC-about 475 BC) derived the notion of regular polyhedra from the shape of a crystal. This legend is not entirely baseless because the southern part in Italy where Pythagoras dwelled and established his school[3] produces Pyrite crystal (an iron sulfide with the formula FeS_2) whose shape is roughly cubic, octahedral, or dodecahedral.

Euclid's *Element*, written around 300 BC and consisting of thirteen volumes, ends up with the classification of regular convex polyhedra; that is, it is shown in the final volume that there are exactly five regular convex polyhedra; say, tetrahedron, cube, octahedron, dodecahedron, and icosahedron (Figure 1). According to Plato's dialogue *Timaeus* written around 360 B.C., the first mathematician who established the classification is Theaetetus, a

[2]Poincaré says "If there were no solid bodies in nature, there would be no geometry".

[3]Pythagorean school in Crotone, a Greek colonial town on the south-eastern coast of Italy, was a religious order in which Pythagoras was a sort of cult figure.

contemporary of Plato[4]. In today's viewpoint, the classification of regular polyhedra is closely related to that of finite subgroups of the orthogonal group $O(3)$, point groups in crystallography ([33]).

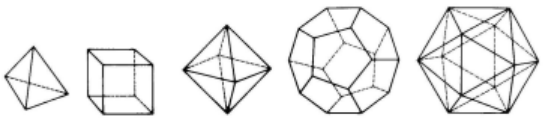

FIGURE 1. Regular convex polyhedra

Pappus (290-350) of Alexandria testifies in his *Collection* that Archimedes (287 BC-212 BC) proposed, in a now-lost work, the notion of *semi-regular polyhedron* as a generalization of regular polyhedron, and found 13 such solids[5]. By this reason, semi-regular polyhedra are sometimes referred to as *Archimedean solids*.

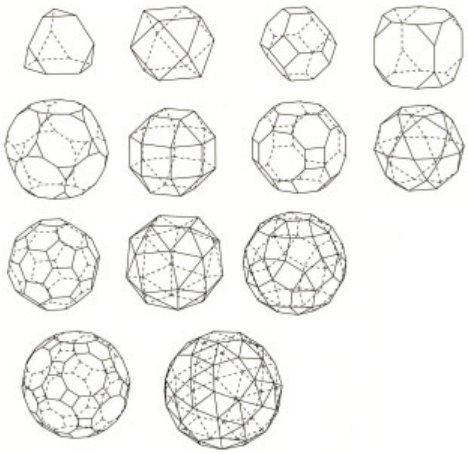

FIGURE 2. Semi-regular convex polyhedra

The discovery of these solids by Archimedes seems to have been made with purely mathematical motivation. After more than 2000 years, however, some of semi-regular polyhedra are going to show up in material science as graphic representations of certain chemical compounds[6].

[4]A regular convex polyhedra, called also Platonic solids, are characterized by the property that its faces are congruent regular polygons, with the same number of faces meeting at each vertex.

[5]A polyhedron is said to be semi-regular if it has regular faces and a symmetry group which is transitive on its vertices. Precisely speaking there are two infinite series of convex prisms and convex antiprisms satisfying this condition.

[6]The network model of Fullerene C_{60}, a compound of carbon atoms whose existence was confirmed in 1990, is the 1-skeleton of the *truncated icosahedron*, one of semi-regular polyhedra.

3. Kepler's contribution to crystallography

Since the period of Hellenism, geometry had taken its own path, and the study of crystals had not been the central theme in mathematics. An exception is the work of Johannes Kepler (1571–1630) on snowflake. Kepler's short pamphlet entitled *New-Year's gift concerning six-cornered snow* ("Strena Seu de Nive Sexangula" in Latin) is considered the first work on the problem of crystal structures[7] though he did not refer to the atomistic viewpoint at all that dates back to ancient Greece[8]. Kepler' motivation came from the question about why snow crystals always exhibit a six-fold symmetry.

Figure 3. Johannes Kepler

Among other things, he pondered two questions in this pamphlet, which are eventually to break new ground in very diverse fields of science, especially in mathematics and crystallography.

(1) He speculated that the densest packing of equally sized spheres is attained by the hexagonal arrangement, which later became known as the Kepler conjecture[9].

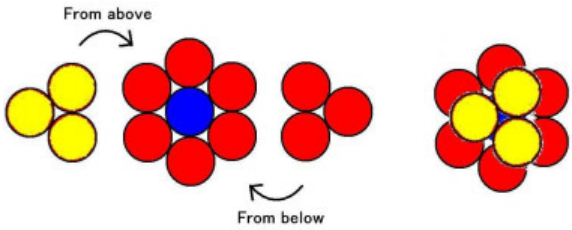

Figure 4. Hexagonal sphere packing

[7]This pamphlet was dedicated on the occasion of the new year of 1611 to his friend and patron, the scholar and imperial privy councilor Johannes Matthäus Wackher von Wackenfels.

[8]The atomism was advocated by Leucippus and Democritus in the 5th century BC.

[9]In 1998 Thomas Hales, following an approach suggested by Fejes Tóth (1953), announced that he had a proof of the Kepler conjecture.

The hexagonal arrangement is closely related to what crystallographers call the *face-centered cubic lattice* (**fcu**[10]) illustrated in Figure 5, where the nodes (vertices) are located at centers of equal spheres, and the line segments (edges) indicate that two spheres located at their end points touch each other.

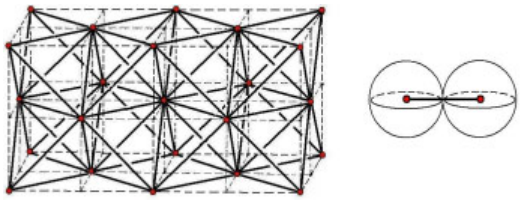

FIGURE 5. The face-centered cubic lattice

(2) In connection with the hexagonal arrangement, Kepler noticed that the honeycomb structure maximizes the number of wax walls each bee shares with his neighbor, thereby allowing bees to collaborate in constructing the shared walls of a cell. The hexagon also turns out to be most efficient in terms of exploiting the maximum of space using the minimal amount of wax[11].

Later we will see that a different kind of minimum principle characterizes the honeycomb structure.

Kepler's observation includes indirect pointers to the law of constant angles for a six-sided snow crystal; thus he is regarded as a forerunner of N. Steno (1669), M. W. Lomonosov (1749) and Romé de l'Isle (1783), the discoverers of the law.

Needless to say, Kepler is renowned as an astronomer who discovered the three laws of planetary motion. His essay demonstrates that Kepler had been thinking of not only the law of the vast universe but also the smallest aspects of nature. It should be emphasized, however, that he was an astrologer and theologian as well, and always sought an interpretation of the harmony of forms as God's choice ([35]). Namely he asks the snowflakes the same question as he did the planets; which form follows God's order.

It is worthwhile to mention that, in *Harmonice Mundi* (1619) which includes his discovery of the third law of planetary motion, Kepler accomplished a complete classification of semi-regular polyhedra ([11]). This achievement tells, though his study on geometric figures can not be separated from his theological dogmatism[12], that he was one of the most outstanding mathematicians of his day.

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[10]We use the three-letter names for crystal ctructures propsed by [34].

[11]Pappus had already noticed that bees have the foresight at their disposal allowing them to understand that a hexagonal partition is more effective than a triangular or a square partition.

[12]It is said that Kepler is the last astronomer of the Renaissance, and not the first of the new age.

4. Crystallographic groups

It is only in the 19th century, more than 2,000 years later since the time of ancient Greece, that mathematics began to play a serious role in crystallography; that is, group theory became matured enough to be applied to the morphology of crystals[13].

As a prehistory of the morphology, there have been observations by people mentioned above about the angles between the faces of a crystal. That is, the faces could be of different sizes, depending upon the conditions under which the crystal have grown, but the relations them remain fixed.

As a reasoning of this fact, Huygens thought of crystals, say the mineral calcite, as being built from small ellipsoidal units (1690). Using this picture, he explained that the resulting faces always preserve the same relationships.

The science of crystallography started when Haiiy published his *Essai d'une Théorie sur la Structure des Cristaux* (1784) in which he developed Huygen's concept to explain the law of angles between faces. Since then, scientists had studied many physical properties (for instance, optical activity discovered by Aragon in 1811) in connection with the morphology of crystals.

The study of morphology led the early crystallographers to a simple classification of all crystals in terms of symmetry. It is German crystallographer J. F. C. Hessel who, for the first time, investigated the possible types of symmetry for a crystal (1830). He found that there are 32 types of groups of symmetry. His book *Krystallonomie und Krystallographie* stating this conclusion was published in Leipzig in 1831, and has not been read seriously enough by other scientists at that time. A. Bravais in 1849 and A. Gadolin in 1867 rediscovered the same 32 symmetry groups by repeating the derivation. Their work was well-known before L. Sohncke, a crystal physicist, found Hessel's earlier book in 1891. It should be pointed out that the notion of groups has been seldom used till 1860'. C. Jordan is the first who recognized that the classification of crystal symmetry is described in terms of subgroups of $O(3)$ (1869). As for 3-dimensional crystallographic groups[14] (space groups), after fundamental works by C. Jordan and L. Sohncke, all 230 isomorphism classes have been determined in 1891 by E. S. Fedorov and A. Schoenflies independently.

From a mathematical viewpoint, it is natural to study crystallographic groups in general dimension. In 1900, D. Hilbert posed a question on finiteness of isomorphism classes of crystallographic groups in his famous address at the second International Mathematical Congress held at Paris. L. Bieberbach (1910-12) and G. Frobenius (1911) solved affirmatively the problem.

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[13]The notion of "group" originated in the work of Evariste Galois (1811-1832) on the inability to generalize the quadratic equation to algebraic equations of degree greater than or equal five. Nowadays the idea of group is one of the great unifying ideas of mathematics.

[14]A subgroup G of the congruence transformation group of $\mathbb{R}^d$ is said to be a d-dimensional crystallographic group if it is discrete and has a compact quotient $G\backslash\mathbb{R}^d$.

5. Discovery of crystal structures

Crystallographic groups introduced to describe macroscopic symmetry of crystals have been a basic tool in classical crystallography even after Max von Laue's discovery of crystal structures by the diffraction of X-rays (1912).

The X-ray technique is based on observing the scattered intensity of an X-ray beam hitting a sample. What was found by Laue is that crystals are solids composed of atoms arranged in an orderly repetitive array, and hence confirmed the anticipation that classical crystallographers had conceived long before. Just after Laue's discovery, W. L. Bragg and W. H. Bragg greatly simplified von Laue's description of X-ray interference, and solved the structures of diamond, sodium chloride (NaCl) and Zinc sulfide (ZnS) in 1913. Today, crystallographers can produce a 3D picture of the density of electrons within the crystal from which the mean positions of the atoms in the crystal can be determined, as well as their mutual interactions.

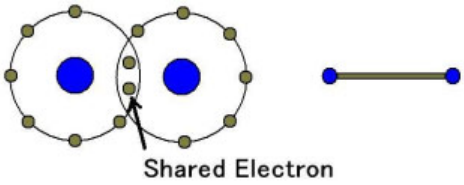

Figure 6. Covalent bonding

It should be worthwhile to point out that there are several ways of interactions. A typical one is *covalent bonding*, which is a form of chemical bonding that is characterized by the sharing of pairs of electrons between atoms (the term "covalent bond" dates from 1939). When we draw a picture of a crystal structure (and any molecule), we join two atoms by a line if they interact each other. This line is called a *bond*.

Let us exhibit a few examples of crystal structures. Figure 7 illustrates the structures of Diamond and Lonsdaleite.

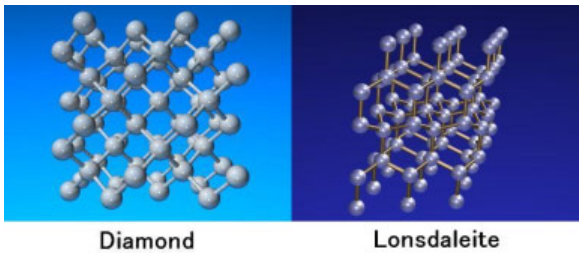

Figure 7. Diamond and Lonsdaleite

Diamond is an allotrope of carbon which is formed and synthesized at high-pressure and high-temperature conditions, and is known to be less stable than graphite[15] though the conversion rate from diamond to graphite is negligible at ambient conditions. Silicon and germanium adopt similar types of crystal structure. On the other hand, Lonsdaleite (called also *hexagonal diamond*) is a carbon allotrope formed when meteorites containing *graphite* strike the Earth, which was first identified in 1967 from the Canyon Diablo meteorite.

The copper crystal is a typical one having the **fcu** structure. Silver and gold also have the **fcu** structure. The honeycomb lattice, a 2D crystal structure, appears as the crystal structure of *Graphene*[16], an allotrope of carbon.

Figure 8 is what crystallographers call the *body-centered cubic lattice* (**bcu**). It is known that the caesium chloride (CsCl) forms a crystal whose structure is **bcu**.

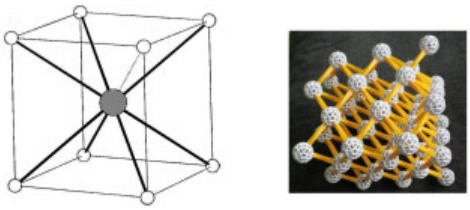

FIGURE 8. The body-centered cubic lattice

We will observe later that the crystal structures mentioned here, say Diamond, Lonsdaleite, **fcu**, **bcu** and honeycomb lattice, share a special feature in view of geometry.

In the 20th century, crystallographer's interest shifted naturally from the morphology of crystals to the study of microscopic crystal structures. As the learned reader may easily conceive, the tool available for this purpose is graph theory, a field studying mathematical structures used to model pairwise relations between objects from a certain collection. Actually one of central themes in modern crystallography is to enumerate (hypothetical) crystals by means of graph theoretic descriptions of crystal structures. Once we find a hypothetical crystal, a systematic prediction of its physical properties for appropriate atoms can be carried out by *first principles calculations*. The prediction by the computer power encourage (or discourage) material scientists to synthesize the hypothetical crystals.

[15]Graphite as a mineral is one of the allotropes of carbon, and the most stable form under standard conditions. It has a layered, planar structure. In each layer, the carbon atoms are arranged in a honeycomb lattice. Weak van der Waals forces hold the layers together.

[16]The term graphene was coined by Hanns-Peter Boehm (1962). The Nobel Prize in Physics for 2010 was awarded to Andre Geim and Konstantin Novoselov "for groundbreaking experiments regarding the two-dimensional material graphene".

Before proceeding to graph theoretic treatment of crystals, let us describe a brief history of the interchange of ideas between chemistry and graph theory.

6. Graphs associated with chemical compounds

A primitive idea of "bond" has been already conceived from as early as the 12th century. It supposes that certain types of *chemical species* are joined by a type of *chemical affinity*. By the mid of 19th century, it was becoming clear that chemical compounds are formed from constituent elements, and the idea of bond had been developed as the theory of *valency* based on the theory of radicals. Especially the theory of chemical structure by the German chemist August Kekulé, in which he took into account the specific combining power (or valences) of specific atoms, provided dramatic new clarity of understanding on chemical compounds (1858).

Here came a fusion of mathematical and chemical ideas. That is, graph theory[17] and chemistry started to interact each other.

Mathematically, a *graph* is represented by an ordered pair $X = (V, E)$ of the set of *vertices* V and the set of all *directed edges* E. Note that each edge has just two directions, which are to be expressed by arrows.

For an directed edge e, we denote by $o(e)$ the *origin*, and by $t(e)$ the *terminus*. The inversed edge of e is denoted by $\overline{e}$. With these notations, we have $o(\overline{e}) = t(e)$, $t(\overline{e}) = o(e)$.

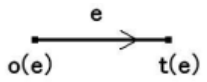

Figure 9. Directed edge

The set of directed edges with origin $x \in V$ is denoted by E_x;

$$E_x = \{e \in E |\ o(e) = x\}.$$

The number of elements in E_x is said to be the *degree* of x, and is denoted by $\deg x$.

The usage of graph theory in chemistry, which is natural in view of the idea of valency, is traced back to 1864 when the Edinburgh chemist Crum Brown proposed to represent chemical compounds by graphs where each atom is represented by a vertex of the graph, and each edge of the graph represents a bond. In 1874, Carl Schorlmmer linked chemistry with trees. Meanwhile French chemist L. Pasteur observed that the relative spatial arrangement of atoms within molecules is vital in understanding of their chemical properties (1861); thus he may be described as the first *stereochemist*. In stereochemistry, molecules are represented as graphs realized in space.

[17]The notion of graphs was implicitly used by Leonhard Euler (1707-1783) when he solved the problem of "Königsberg seven bridges" (1736).

It is interesting to point out that the term "graph" was used for the first time by Sylvester in a note appeared in the scientific journal *Nature* (1878) where a relationship between chemistry and algebra was suggested.

To avoid a confusion, we shall use the terminology "network" (or simply "net") from now on when we are handling a graph placed in space (plane).

7. Fundamental finite graphs and building blocks

After confirmed that atoms and molecules have physical existence, network representations of molecules also broke away from fictitious entity. It is thus a matter of course for crystallographers to employ graph theory for the study of crystal structures. Strangely enough, however, the systematic approach by means of graph theory has not been done until 1950's though, by this time, plenty of crystal structures have been understood and represented by networks. The reason may be due to the self-explanatory fact that the ideal model of a crystal is an *infinite* graph, which is not an object that the ordinary graph theory handles.

It is A. F. Wells who initiated the intensive research by treating crystals as *periodic* 3D nets in space ([41], [42]). In his influential book [42] (1977), Wells treated *uniform* nets, and tried to investigate them systematically. Here "uniform" means that the net is a regular graph, and that the shortest circuit containing any two edges through any vertex shall have the same number of edges.

The net associated with a crystal is not just an infinite graph realized in space (or plane), but, as observed by crystallographers ([8]), a graph with a translational action which becomes a finite graph when factored out. We shall take up the term "a Bravais lattice" to express a group of translations leaving the crystal invariant. The finite graph obtained by factoring out is called the *fundamental finite graph* (or quotient graph). This observation has been used in a systematic enumeration of crystal structures (see [24] for instance).

To illustrate the concrete way to get the fundamental finite graph $X_0 = (V_0, E_0)$ from a net $X = (V, E)$ of a crystal, we employ Figure 10. Here as a Bravais lattice, we take the lattice group generated by two vectors depicted by arrows. We first label vertices and edges of X; say, A, B, C, D for vertices and a, b, c, d, e, f for edges in the honeycomb lattice, in such a way that the same label is assigned to two edges (resp. two vertices) if one is obtained from another by a translation belonging to the Bravais lattice. Then we gather the labels of vertices and join them by labeled edges, keeping the adjacency relation. Thus one gets the fundamental finite graph[18].

This construction allows us to assign a vector $\mathbf{v}(e)$ to each directed edge e in X_0 as follows. Choose a direct edge e' in X which corresponds to e.

[18]What we explained here is a special case of the construction of *quotient sets* associated with *equivalence relations*.

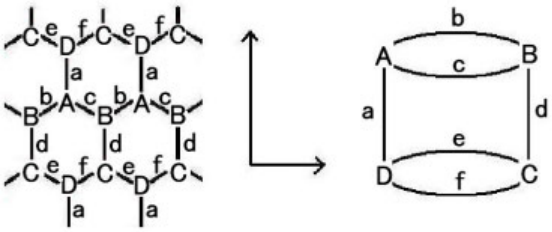

FIGURE 10. How to get the fundamental finite graph

Since e' is a directed line segment in space (or plane), it represents a vector $\mathbf{v}(e)$ which does not depend upon the choice of e'. Obviously $\mathbf{v}(\overline{e}) = -\mathbf{v}(e)$.

The system of vectors

$$\{\mathbf{v}(e)\}_{e\in E_0} = \bigcup_{x\in V_0} \{\mathbf{v}(e)|\ e \in E_{0x}\}$$

completely determines the net X. In this sense, $\{\mathbf{v}(e)\}_{e\in E_0}$ deserves to be called the *building block*[19] of X.

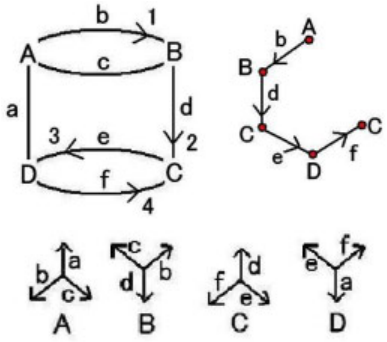

FIGURE 11. A building block

Figure 11 tells how to get the crystal from the building block. For example, travel on the graph X_0 along $AbBdCeDfC$, and sum up the vectors corresponding to directed edges in the trail[20]

$$\overrightarrow{AbB} + \overrightarrow{BdC} + \overrightarrow{CeD} + \overrightarrow{DfC}.$$

Drawing such vector sums in plane for all trails starting from A, we obtain the honeycomb X.

Again from the construction of the fundamental finite graph, we obtain a map from X onto X_0 in a natural manner, which we call the *canonical map* (precisely speaking, the canonical map is a *morphism* of graphs which

[19]Crystallographers use the term "a labelled quotient graph" for X_0 with a building block. Mathematically a building block is nothing but a 1-cochain on X_0 with values in $\mathbb{R}^d$.

[20]In Section 8, "trails" will be called "paths".

brings vertices to vertices and edges to edges in such a way that the adjacency relation between vertices and edges is preserved.

One should remark that the choice of Bravais lattice is not unique. Two Bravais lattices (represented by arrows) are shown in the Figure 12. The corresponding fundamental finite graphs are depicted on the left and right. We usually take the maximal one as a Bravais lattice.

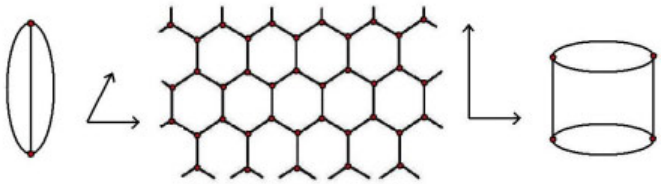

FIGURE 12. Two Bravais lattice and their fundamental finite graphs

We now take a look at Diamond and Lonsdaleite. For Diamond, if we take the maximal Bravais lattice, the fundamental finite graph is the graph (A) in Figure 13 consisting of two vertices joined by four parallel edges[21]. For Lonsdaleite, its fundamental finite graph is the graph (B). In both cases, the building blocks are related to the regular tetrahedron.

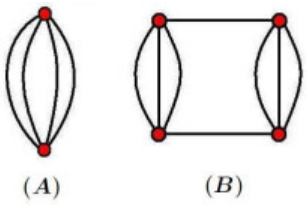

FIGURE 13. Fundamental finite graphs for Diamond and Lonsdaleite

Figure 14 is the crystal structure of the 3D *kagome lattice*[22], which is comprised of corner-sharing tetrahedra. The fundamental graph for the maximal Bravais lattice is given on the right. The 3D kagome lattice turns out to have a special feature as seen in Section 13.

It is interesting to point out that 1-skeletons of many semi-regular polyhedra are hidden in crystals. For instance, one can find the cubooctahedron in the face-centered cubic lattice, and truncated tetrahedron in the 3D kagome lattice.

So far we have traced the path that crystallographers have taken. Now let us ask a mathematician "What's the mathematical nature of crystal structures ?". His immediate answer would be "Topologically they are infinite-fold abelian covering graphs over finite graphs. Crystals are their periodic

[21]The honeycomb lattice is considered the 2-dimensional analogue of the diamond crystal

[22]This is a 3D version of the ordinaly kagome lattice; see Section 13.

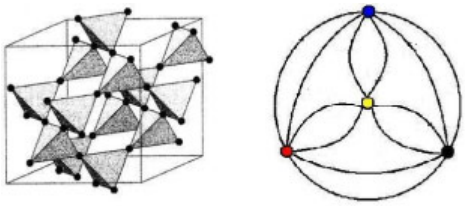

FIGURE 14. 3D kagome lattice and its fundamental finite graph

realizations in space". This simple answer is a sort of folklore in the community of mathematicians, and hence it is not attributed to anybody. It is no wonder, however, that Henri Poincaré (1854-1912), founder of algebraic topology, could have easily conceived this answer if he would have witnessed Laue's discovery, which was coincidentally accomplished in the last year of Poincaré's life.

The main aim from now on is to explain the nature of this answer by adopting routine tools in algebraic topology.

8. Homology

The homology group (of a cell complex in general) is an algebraic system constructed from figures (cells)[23]. We are not going to be involved in its general theory, but shall confine ourselves to the case of graphs. The reader who is familiar with algebraic topology may skip the definitions of homology groups and covering graphs.

Given a finite graph $X_0 = (V_0, E_0)$, we consider a sum over vertices of the following form

$$\sum_{x \in V_0} a_x x \qquad (a_x \in \mathbb{Z}).$$

We call such a sum a 0-*chain* (with coefficients in $\mathbb{Z}$). This sum and the product $a_x x$ (*integer* $\times$ *vertex*) are formal so that one should not worry about their meaning. The set of 0-chains is denoted by $C_0(X, \mathbb{Z})$ with which we equip the structure of a free abelian group in the following way.

(1) $\displaystyle\sum_{x \in V_0} a_x x = 0$ if and only if $a_x = 0$ for every $x \in V_0$,

(2) $\displaystyle\sum_{x \in V_0} a_x x \pm \sum_{x \in V_0} b_x x = \sum_{x \in V_0} (a_x \pm b_x) x.$

Thus $C_0(X, \mathbb{Z})$ is a free abelian group with the $\mathbb{Z}$-basis V.

Likewise we define the abelian group $C_1(X_0, \mathbb{Z})$ consisting of finite formal sums over directed edges

$$\sum_{e \in E_0} a_e e \qquad (a_e \in \mathbb{Z}),$$

[23]Historically the germination of homology theory is seen in the work by Riemann and Poincaré on algebraic functions.

which we call a 1-*chain* (with coefficients in $\mathbb{Z}$). In this turn, however, we impose the relation $\overline{e} = -e$ so that a way to express a 1-chain as above is not unique[24]. If we fix an orientation E_0^o of X; that is, a subset $E_0^o \subset E_0$ satisfying $E_0^o \cap \overline{E_0^o} = \emptyset$, $E_0^o \cup \overline{E_0^o} = E_0$, then E_0^o is a $\mathbb{Z}$-basis of $C_1(X_0, \mathbb{Z})$, so that any 1-chain is expressed as $\sum_{e \in E_0^o} a_e e$ in a unique way.

Roughly speaking, the homology group of a graph is introduced to describe the adjacency relation between vertices and edges in an algebraic way. To be exact, we define the *boundary operator* (homomorphism) $\partial : C_1(X_0, \mathbb{Z}) \longrightarrow C_0(X_0, \mathbb{Z})$ by putting $\partial(e) = t(e) - o(e)$ and extending it to a homomorphism, where we should note that $\partial\overline{e} = \partial(-e)$, and hence the definition of ∂ is compatible with the relation $\overline{e} = -e$. The 1-homology group $H_1(X_0, \mathbb{Z})$ is defined to be the kernel of ∂:

$$H_1(X_0, \mathbb{Z}) = \mathrm{Ker}\ \partial\ (= \{\alpha \in C_1(X_0, \mathbb{Z}) |\ \partial\alpha = 0\}).$$

An element of $H_1(X_0, \mathbb{Z})$ is said to be a *homology class* or a 1-cycle. $H_1(X_0, \mathbb{Z})$ is a free abelian group of finite rank. The rank of $H_1(X_0, \mathbb{Z})$, symbolically $b_1(X_0)$, is called the (first) *Betti number*. The Betti number is an indicator of the "complexity" of finite graphs.

Homology classes are represented by closed paths. Here a *path* in X_0 is a sequence of edges $c = (e_1, \ldots, e_n)$ with $t(e_i) = o(t_{i+1})$ $(i = 1, \ldots, n-1)$. If $t(e_n) = o(e_1)$, then c is said to be *closed*.

FIGURE 15. A path

For a path $c = (e_1, \ldots, e_n)$ in X_0, the symbol $\langle c \rangle$ expresses the 1-chain $e_1 + \cdots + e_n$. If c is closed, then $\partial(e_1 + \cdots + e_n) = 0$, and hence $\langle c \rangle$ is a homology class. An important fact we frequently use is that *every homology class is represented by a closed path*.

We shall enumerate several facts of the homology group.

Fact 1 There exists a $\mathbb{Z}$-basis of $H_1(X_0, \mathbb{Z})$ consisting of homology classes represented by closed paths.

Fact 2 Let T ba a spanning tree[25] in X_0. Then the number of undirected edges in X_0 not contained in T is equal to the first Betti number $b_1(X_0)$.

---

[24]We are considering the factor group of the free abelian group with the $\mathbb{Z}$-basis E_0 modulo the subgroup generated by $\{e + \overline{e} |\ e \in E_0\}$.

[25]Among all subtrees in a graph X_0, we can find a maximal one with respect to inclusion, which we call a spanning tree of X_0.

Fact 3 When X_0 is a *plane graph*[26] without vertices of degree one, X_0 divides the plane into a finitely many bounded connected small regions; say, $D_1, \dots, D_k$. One can prove $k = b_1(X_0)$.

Fact 4 (The Euler relation) $|V_0| - |E_0|/2 = 1 - b_1(X_0)$. This is equivalent to Euler's polyhedral theorem[27].

Given a system of vectors $\{\mathbf{v}(e)\}_{e\in E_0}$, we consider the homomorphism

$$\widehat{\mathbf{v}} : H_1(X_0, \mathbb{Z}) \longrightarrow \mathbb{R}^d \quad (d = 2, 3)$$

defined by

$$\widehat{\mathbf{v}}\Big(\sum_{e\in E_0} a_e e\Big) = \sum_{e\in E_0} a_e \mathbf{v}(e).$$

One can easily check that $\widehat{\mathbf{v}}$ is well-defined, and that, if $\{\mathbf{v}(e)\}_{e\in E_0}$ is a building block of a crystal, then the image $\widehat{\mathbf{v}}(H_1(X_0, \mathbb{Z}))$ coincides with the Bravais lattice. The converse holds:

Theorem 8.1. *A system of vectors $\{\mathbf{v}(e)\}_{e\in E_0}$ in $\mathbb{R}^d$ is a building block of a crystal if and only if the image of $\widehat{\mathbf{v}}$ is a lattice group in $\mathbb{R}^d$*

The proof is given in the next section.

So far we have handled the homology group with coefficients in $\mathbb{Z}$. In a similar fashion, $H_1(X_0, \mathbb{R})$, the 1-homology group with coefficients in $\mathbb{R}$, is defined by replacing $\mathbb{Z}$ by $\mathbb{R}$ in the definition. The group $H_1(X_0, \mathbb{R})$ is actually a vector space over $\mathbb{R}$, and $H_1(X_0, \mathbb{Z})$ is a lattice group in $H_1(X, \mathbb{R})$.

9. Topological crystals

Recall that, given the net X associated with a crystal and a Bravais lattice, we have the canonical map $\omega : X \longrightarrow X_0$. A special feature of ω is that it is a *regular covering map*[28] whose covering transformation group is isomorphic to $\mathbb{Z}^d$ $(d = 2, 3)$.

For the convenience of the reader, let us give a graph-theoretical description of maps between graphs, and also covering maps. Let $X = (V, E)$, $X_0 = (V_0, E_0)$ be connected graphs. A morphism $\omega : X \longrightarrow X_0$ is a correspondence of vertices and edges preserving the adjacency relation among them. More precisely, it is a pair $\omega = (\omega_V, \omega_E)$ of maps $\omega_V : V \longrightarrow V_0$, $\omega_E : E \longrightarrow E_0$ satisfying $o\big(\omega_E(e)\big) = \omega_V\big(o(e)\big)$, $t\big(\omega_E(e)\big) = \omega_V\big(t(e)\big)$ for every

[26] A plane graph is a graph drawn on the plane in such a way that its edges intersect only at their endpoints, while a *planar graph* is a graph that *can be* embedded in the plane.

[27] This theorem due to Euler (1750) asserts $v - e + f = 2$ where v, e, f are the number of vertices, edges and faces of a convex polyhedron. One can make use of this formula to prove that there are just 5 regular convex polyhedra. Historically Euler's theorem is considered to be the starting point of "topology".

[28] A primitive idea of covering maps for general spaces is seen in Riemann's study of algebraic functions and their integrals (1851). The book Lehrbuch der Topologie by H. Seifert and W. Threlfall published in 1934 gave a rigorous set-up and popularized the notion of covering maps.

$e \in E$, and $\overline{\omega_E(e)} = \omega_E(\overline{e})$. By abuse of notations, we write $\omega(x)$ for $\omega_V(x)$ and $\omega(e)$ for $\omega_E(e)$ for simplicity.

If both ω_V and ω_E are bijective (one-to-one and onto), the morphism $\omega = (\omega_V, \omega_E)$ is said to be an *isomorphism.* An isomorphism ω of X onto itself is called an *automorphism.* The totality of automorphisms of X, symbolically $\mathrm{Aut}(X)$, is a group in a natural manner.

A morphism $\omega : X \longrightarrow X_0$ is said to be a *covering map* if

(i) $\omega : V \longrightarrow V_0$ is surjective,

(ii) for every $x \in V$, the restriction $\omega|E_x : E_x \longrightarrow E_{0,\omega(x)}$ is a bijection.

The group $G(\omega) = \{\sigma \in \mathrm{Aut}(X) |\ \omega \circ \sigma = \omega\}$ is called the *covering transformation group* of the covering map ω. A covering map ω is said to be *regular* if, for any $x, y \in V$ with $\omega(x) = \omega(y)$, there exists an element $\sigma \in G(\omega)$ such that $y = \sigma x$.

Let d be any positive integer. A d-dimensional *topological crystal*[29] X is a regular covering graph over a *finite graph*, say X_0, whose covering transformation group L is a free abelian group of rank d. After the case of the net associated with a crystal, we call X_0 the fundamental finite graph. X (or $\omega : X \longrightarrow X_0$) is said to be a topological crystal over X_0. We also call L an *abstract Barvais lattice.*

In a word, a topological crystal is an abstraction of a real crystal, the notion obtained by forgetting how the net are placed in space, which, however, still retains all the information on the connectivity of atoms in the crystal.

The following is well-known in the general theory of covering maps:

Theorem 9.1. (1) *There exists a (unique) topological crystal* $\omega^{\mathrm{ab}} : X_0^{\mathrm{ab}} \longrightarrow X_0$ *such that the dimension of* X_0^{ab} *is* $b_1(X_0)$*. Its abstract Bravais lattice is* $H_1(X_0, \mathbb{Z})$*.*

(2) *For any topological crystal* $\omega : X \longrightarrow X_0$*, there exists a regular bcovering map* $\omega_1 : X_0^{\mathrm{ab}} \longrightarrow X$ *such that* $\omega \circ \omega_1 = \omega^{\mathrm{ab}}$ (ω_1 *is called a subcovering map*)*. The dimension of* X *is less than or equal to* $b_1(X_0)$*. In this sense,* X_0^{ab} *is the maximal one*[30] *among all topological crystals over* X_0*. We shall calle* X_0^{ab} *the maximal topological crystal over* X_0*.*

(3) *The covering transformation group* H *of* $\omega_1 : X_0^{\mathrm{ab}} \longrightarrow X$ *is a subgroup of* $H_1(X_0, \mathbb{Z})$ *such that the factor group* $H_1(X_0, \mathbb{Z})/H$ *is isomorphic to the abstract Bravais lattice of topological crystal* $\omega : X \longrightarrow X_0$ *and hence free abelian. Conversely, for a subgroup* H *of* $H_1(X_0, \mathbb{Z})$ *such that* $H_1(X_0, \mathbb{Z})/H$ *is free abelian, there exists a topological crystal* X *whose abstract Bravais lattice is* $H_1(X_0, \mathbb{Z})/H$*.*

[29]The reason to adopt the term "topological crystal" is to emphasize its abstract nature and at the same time to keep the word "crystal" in order to make it clear that we are addressing the problem of crystals, not the problem of general graphs. Chemical crystallographers adopt the term " periodic graphs " for the underlying topology of crystal structures.

[30]In [4], the term "minimal net" is used for the maximal abelian covering over a finite graph.

A subgroup H of $H_1(X_0, \mathbb{Z})$ such that the factor group $H_1(X_0, \mathbb{Z})/H$ is free abelian will be called a *vanishing subgroup*.

Roughly speaking, the theorem above tells that there is a one-to-one correspondence between the family of topological crystals X over X_0 and the family of vanishing subgroups H of $H_1(X_0, \mathbb{Z})$.

As an example of X_0, let us consider the 3-*bouquet graph* B_3 (Figure 16)[31]. Let $E_0^o = \{e_1, e_2, e_3\}$ be an orientation of B_3. Then, e_1, e_2, e_3 constitute a $\mathbb{Z}$-basis of $H_1(B_3, \mathbb{Z})$. The maximal topological crystal over B_3 is the (topological) cubic lattice. On the other hand, the *triangular lattice* is a topological crystal corresponding to the vanishing subgroup $H = \mathbb{Z}(e_1 + e_2 + e_3)$.

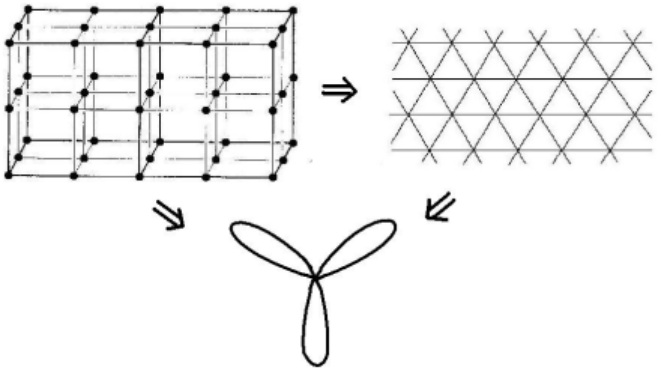

FIGURE 16. The cubic lattice and the triangular lattice

We now give a proof of Theorem 8.1. Let $H = \{\alpha \in H_1(X_0, \mathbb{Z}) | \ \widehat{\mathbf{v}}(\alpha) = 0\}$, the kernel of $\widehat{\mathbf{v}}$, and $\omega : X \longrightarrow X_0$ be the topological crystal corresponding to H. Define the map $\Phi : V \longrightarrow \mathbb{R}^d$ by setting

$$\Phi(x) = \mathbf{v}(\omega(e_1)) + \cdots + \mathbf{v}(\omega(e)),$$

where $c = (e_1, \ldots, e_n)$ is a path in X joining a reference point x_0 and x (one can prove that $\Phi(x)$ does not depend upon the choice of c). Then we extend Φ to a piecewise linear map from X into $\mathbb{R}^d$. The reader may notice that the definition of Φ is a generalization of what we have illustrated in Section 7 for the honeycomb lattice. The crystal which we wanted is defined as the image of Φ.

One can check

$$\mathbf{v}(\omega(e)) = \Phi(t(e)) - \Phi(o(e))$$

and

$$\Phi(\sigma x) = \Phi(x) + \rho(\sigma), \tag{1}$$

where σ is an arbitrary element of the abstract Bravais lattice $L = H_1(X_0, \mathbb{Z})/H$, and $\rho : L \longrightarrow \mathbb{R}^d$ is the injective homomorphism characterized by $\widehat{\mathbf{v}}(\alpha) =$

[31]The n-bouquet graph is the graph with a single vertex with n loop edges.

$\rho(\mu(\alpha))$. Here $\mu : H_1(X_0, \mathbb{Z}) \longrightarrow L = H_1(X_0, \mathbb{Z})/H$ is the canonical homomorphism.

10. Enumeration of topological crystals

If we forget how crystals are placed in space, then the enumeration of crystals reduces to that of topological crystals, or equivalently the enumeration of finite graphs X_0 and vanishing subgroups H of $H_1(X_0, \mathbb{Z})$.

If we restrict ourselves to the class of finite graphs X_0 such that $\deg x \geq 3$ for every $x \in V_0$, then there are only finitely many X_0 with a fixed Betti number. Thus one can enumerate X_0 in principle at least.

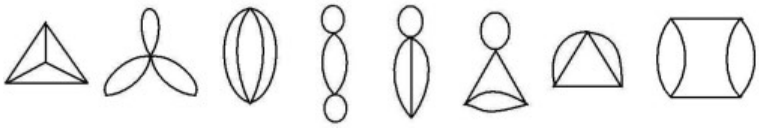

Figure 17. Several graphs with $b_1 = 3$

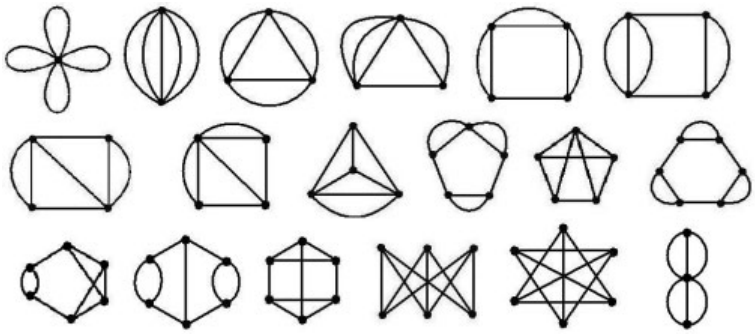

Figure 18. Several graphs with $b_1 = 4$

It should be pointed out that, given an integer d with $1 \leq d < b_1(X_0)$, there are infinitely many vanishing groups H with rank $H_1(X_0, \mathbb{Z})/H = d$, from which it follows that there are infinitely many d-dimensional topological crystals over X_0. Hence to enumerate topological crystals, we need to introduce a sort of "magnitude" of vanishing subgroups H. For this sake, we first define the norm $\|\alpha\|_1$ of a 1-chain $\alpha = \sum_{e \in E_0^o} a_e e$ by setting

$$\|\alpha\|_1 = \sum_{e \in E_0^o} |a_e|,$$

where it should be noted that $\|\alpha\|_1$ does not depend upon the choice of an orientation E_0^o. Then for a $\mathbb{Z}$-basis $S = \{\alpha_{d+1}, \ldots, \alpha_b\}$ of a vanishing subgroup H, we put

$$h(S) = \max(\|\alpha_{d+1}\|_1, \ldots, \|\alpha_b\|_1),$$

and define the *height* of H by

$$h(H) = \min_S h(S).$$

Consider two sets

$$R_1 = \{S|\ h(S) \leq h\},$$
$$R_2 = \{H|\ h(H) \leq h\}.$$

Clearly R_1 is a finite set. The correspondence

$$S \mapsto H \text{ generated by S}$$

gives a surjective map of R_1 onto R_2. Thus we get the following:

Theorem 10.1. *For any positive number h and positive integer d with $1 \leq d < b_1(X_0)$, there are only finite number of vanishing subgroups H of $H_1(X_0, \mathbb{Z})$ satisfying*

(1) $\operatorname{rank} H_1(X_0, \mathbb{Z})/H = d$,

(2) $h(H) \leq h$.

11. Canonical placements

Topological crystals are purely mathematical objects "living in the logical world, but not in real space" in the sense that they are constructed on the basis of pure reflection[32], thereby being not visible even for the 3D case if we would leave it intact.

The issue of topological crystals becomes more interesting if we seek the most natural way to place them in space. For instance, the diamond crystal is one of the placements in space of the topological diamond (the maximal topological crystal over the graph (A) in Figure 13). Figure 19 illustrates another placement of the topological diamond ("graphite-like" placement).

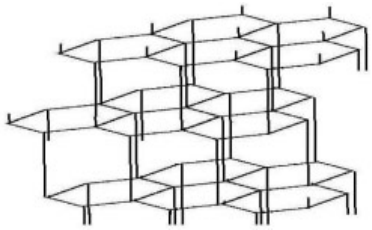

Figure 19. The graphite-like placement of the diamond crystal

Actually there are infinitely many ways to realize a given topological crystal in space. Then a natural question is raised: "what is the most canonical placement, especially what are the characteristics possessed by

[32]This is the so-called *Platonic view*; that is, we mathematicians insist that mathematical entities are abstract in not being spatiotemporally located, and hence lie outside a real world.

the diamond crystal that differ from all other placements of the topological diamond ?"

The diamond crystal is more symmetric than its graphite-like placement. This observation motivates us to seek the most symmetric placements in general. As a candidate of such placements, we shall introduce the notion of *canonical placements* (see Remark below).

We first define the notion of general placements in view of (1). Let $X = (V, E)$ be a d-dimensional topological crystal with an abstract Bravais lattice L, and let $X_0 = (V_0, E_0)$ be its fundamental finite graph. A piecewise linear map $\Phi : X \longrightarrow \mathbb{R}^d$ is said to be a *placement* if there exists an injective homomorphism $\rho : L \longrightarrow \mathbb{R}^d$ satisfying

(1) $\Phi(\sigma x) = \Phi(x) + \rho(\sigma) \qquad (x \in V,\ \sigma \in L)$,

(2) $\rho(L)$ is a lattice subgroup of $\mathbb{R}^d$.

The image $\Phi(X)$ is the cystal[33] associated with the topological crystal X. Its Bravais lattice is $\rho(L)$. The building block $\{\mathbf{v}(e)\}_{e\in E_0}$ of $\Phi(X)$ is given by $\mathbf{v}(\omega(e)) = \Phi(t(e)) - \Phi(o(e))$. As in the case of nets, the building block determines Φ uniquely (up to translations).

To define the canonical placement of X, we shall resort to a certain minimal principle, having in mind Euler's remark "Since the fabric of the Universe is most perfect and the work of a most wise creator, nothing at all takes place in the Universe in which some rule of maximum or minimum does not appear".

In order to formulate the minimal principle, let us think of a crystal as a system of *harmonic oscillators*; that is, each edge is supposed to represent a harmonic oscillator whose energy is the square of its length (Figure 20). This simple model of a crystal leads us to the notion of *energy* functional defined as[34]

$$E(\Phi) = \mathrm{vol}\big(D_{\rho(L)}\big)^{-2/d} \sum_{e\in E_0} \|\mathbf{v}(e)\|^2, \tag{2}$$

which is regarded as the "normalized" total potential energy of the system *per unit cell*. Here $\mathrm{vol}\big(D_{\rho(L)}\big)$ stands for the volume of the unit cell $D_{\rho(L)}$ associated with the Bravais lattice $\rho(L)$.

The presence of the term $\mathrm{vol}\big(D_{\rho(L)}\big)^{-2/d}$ in (2) makes $E(\Phi)$ a size-free quantity.

The *canonical placement* is defined to be a placement Φ minimizing $E(\Phi)$.

---

[33]Strictly speaking, $\Phi(X)$ could be pathological in the sense that different vertices may be mapped by Φ to the same point, the image of an edge may collapse, or the image of two edges may overlap.

[34]A real crystal (crystalline solid) is also physically regarded as a system of harmonic oscillators under an appropriate approximation of the equation of motion, but the shape of energy is much more complicated.

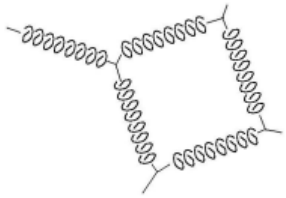

FIGURE 20. A system of harmonic oscillators

Theorem 11.1. ([30],[27]) (1) *There exists a unique canonical placement Φ of E up to homothetic transformations*[35] *of $\mathbb{R}^d$.*

(2) *A placement Φ is canonical if and only if*

$$\sum_{e\in E_{0x}} \mathbf{v}(e) = \mathbf{0} \qquad (x \in V_0), \tag{3}$$

$$\sum_{e\in E_0} \langle \mathbf{v}(e), \mathbf{n}\rangle^2 = c \text{ (constant)} \tag{4}$$

for any unit vector $\mathbf{n} \in \mathbb{R}^d$,

One can see that (5) is equivalent to there being a positive constant c such that, for any $\mathbf{x} \in \mathbb{R}^d$,

$$\sum_{e\in E_0} \big\langle \mathbf{x}, \mathbf{v}(e)\big\rangle \mathbf{v}(e) = c\mathbf{x}. \tag{5}$$

Namely (5) is equivalent to saying that $\{\mathbf{v}(e)\}_{e\in E_0}$ is a *tight frame*, a notion introduced in wavelet analysis.

The condition (3) in the theorem tells that the crystal as a system of harmonic oscillators is in equilibrium in the sense that the total force acting on any "atom" from its nearest neighbors vanishes. A placement satisfying (3) is what we called a *harmonic realization* in [27] because (3) is equivalent to saying that Φ is "harmonic" with respect to the discrete version of the Laplacian ([39], [28], [30]); see Remark (2) in the next section.

The proof for the characterization (3), (4) in Theorem 11.1 relies on the following fact:

For a symmetric matrix S of size d with positive eigenvalues,

$$\operatorname{tr} S \geq d(\det S)^{1/d}, \tag{6}$$

where the equality holds if and only if S is a scalar matrix, i.e. $S = \lambda I_d$ with $\lambda > 0$. The inequality (6) reduces to the *inequality of arithmetic and*

[35] A *homothetic transformation* of $\mathbb{R}^d$ is an affine transformation of the form

$$M(\mathbf{x}) = cU\mathbf{x} + \mathbf{a} \qquad (c > 0,\ \mathbf{a} \in \mathbb{R}^d),$$

where U is an orthogonal matrix, i.e. $U \in O(d)$. A *congruent transformation* is the case that $c = 1$.

geometric means:

$$\frac{1}{d}(a_1 + \cdots + a_d) \geq (a_1 \cdots a_d)^{1/d}.$$

The existence of canonical placements will be shown in the next section.

In the case of maximal topological crystals, we have the following explicit inequality

$$E(\Phi) \geq 2b_1(X_0)\kappa(X_0)^{-1/b_1(X_0)},$$

where $\kappa(X_0)$ is the number of spanning trees in X_0. The equality holds if and only if $\Phi = \Phi^{\mathrm{ab}}$ (up to homothety).

The following theorem tells that the canonical placement has the property "extrinsic symmetry =intrinsic symmetry", and hence has *maximal symmetry* among all placement[36].

Theorem 11.2. ([30]) *Let $\Phi : X \longrightarrow \mathbb{R}^d$ be the canonical placement. Then there exists a homomorphism $\kappa : \mathrm{Aut}(X) \longrightarrow M(d)$ such that*

(1) *when we write $\kappa(g) = \big(A(g), b(g)\big) \in O(d) \times \mathbb{R}^d$, we have*

$$\Phi(gx) = A(g)\Phi(x) + b(g) \qquad (x \in V),$$

(2) *the image $\kappa\big(\mathrm{Aut(X)}\big)$ is a crystallographic group,*

12. Construction of canonical placements

The canonical placement of the maximal topological crystal X_0^{ab} is constructed in the following way. First we provide $H_1(X_0, \mathbb{R})$, the 1-homology group with real coefficients, with a natural inner product (which allows us to identify $H_1(X_0, \mathbb{R})$ with the Euclidean space $\mathbb{R}^b$, $b = b_1(X_0)$). For this sake, we start with an inner product on $C_1(X_0, \mathbb{R})$, the group of 1-chains with real coefficients.

For $e, e' \in E_0$, we set

$$\langle e, e' \rangle = \begin{cases} 1 & (e' = e) \\ -1 & (e' = \overline{e}) \\ 0 & (\text{otherwise}) \end{cases},$$

which extends to an inner product on $C_1(X_0, \mathbb{R})$ in a natural manner; say,

$$\Big\langle \sum_{e \in E_0} a_e e, \sum_{e \in E_0} b_{e'} e' \Big\rangle = \sum_{e, e' \in E_0} a_e b_{e'} \langle e, e' \rangle.$$

Restricting this inner product to the subspace $H_1(X_0, \mathbb{R})$ ($= \mathrm{Ker}\, \partial \subset C_1(X_0, \mathbb{R})$), we get an Euclidean structure on $H_1(X_0, \mathbb{R})$, which will be the space where the maximal topological crystal X_0^{ab} is placed.

[36]Roughly speaking, maximal symmetry means that no structural deformation of its periodic arrangement of atoms in a crystal will make the structure more symmetrical than it is

Let $P_{\mathrm{ab}} : C_1(X_0, \mathbb{R}) \longrightarrow H_1(X_0, \mathbb{R})$ be the orthogonal projection, and put $\mathbf{v}_{\mathrm{ab}}(e) = P_{\mathrm{ab}}(e)$, regarding each edge as a 1-chain. Since $\widehat{\mathbf{v}}^{\mathrm{ab}} : H_1(X_0, \mathbb{Z}) \longrightarrow H_1(X_0, \mathbb{R})$ coincides with the injection, it follows from Theorem 8.1 that $\mathbf{v}_{\mathrm{ab}}(e)\}_{e \in E_0}$ is a building block of a placement Φ^{ab} of the maximal topological crystal X_0^{ab}. One can prove that Φ^{ab} is canonical.

We now go over to the general case. Let X be a topological crystal over X_0 corresponding to a vanishing subgroup H of $H_1(X_0, \mathbb{Z})$. Let $H_{\mathbb{R}}$ be the subspace of $H_1(X_0, \mathbb{R})$ spanned by H, and $H_{\mathbb{R}}^{\perp}$ the orthogonal complement of $H_{\mathbb{R}}$ in $H_1(X_0, \mathbb{R})$:

$$H_1(X_0, \mathbb{R}) = H_{\mathbb{R}} \oplus H_{\mathbb{R}}^{\perp}.$$

Then $\dim H_{\mathbb{R}}^{\perp} = \operatorname{rank} L = d$. By choosing an orthonormal basis of $H_{\mathbb{R}}^{\perp}$, we identify $H_{\mathbb{R}}^{\perp}$ with the Euclidean space $\mathbb{R}^d$.

Let $P : H_1(X_0, \mathbb{R}) \longrightarrow H_{\mathbb{R}}^{\perp} = \mathbb{R}^d$ be the orthogonal projection. If we put $\mathbf{v}(e) = P\big(\mathbf{v}_{\mathrm{ab}}(e)\big)$, then we find that $\{\mathbf{v}(e)\}_{e \in E_0}$ gives the building block of the canonical placement of X.

To sum up, we have the following commutative diagram for the canonical placements.

$$\begin{array}{ccc} X_0^{\mathrm{ab}} & \xrightarrow{\Phi^{\mathrm{ab}}} & \mathbb{R}^b \\ {\scriptstyle \omega_1}\big\downarrow & & \big\downarrow{\scriptstyle P} \\ X & \xrightarrow[\Phi]{} & \mathbb{R}^d \end{array}$$

i.e., $P \circ \Phi^{\mathrm{ab}} = \Phi \circ \omega_1$, where $\omega_1 : X_0^{\mathrm{ab}} \longrightarrow X$ is the subcovering map of $\omega^{\mathrm{ab}} : X_0^{\mathrm{ab}} \longrightarrow X_0$. To coin a phrase, the canonical placement of a topological crystal is obtained by projecting down the canonical placement of the maximal topological crystal onto a suitable hyperplane.

Finally we shall give a practical procedure by means of matrix computations to materialize the logically constructed object, thereby giving a powerful approach to the systematic design of (hypothetical) crystal structures.

(1) Give a finite graph X_0, and a vanishing subgroup H of $H_1(X_0, \mathbb{Z})$. Take a $\mathbb{Z}$-basis $\alpha_1, \ldots, \alpha_b$ ($b = b_1(X_0)$) of $H_1(X_0, \mathbb{Z})$ such that $\alpha_{d+1}, \ldots, \alpha_b$ ($d \leq b$) comprise a $\mathbb{Z}$-basis of H. We then have the d-dimensional topological crystal X corresponding to H.

(2) Compute the square matrix of size b

$$A = \big(\langle \alpha_i, \alpha_j \rangle\big) = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

where A_{11} (resp. A_{22}) is a square matrix of size d (resp. $b - d$).

Put $\Gamma = A_{11} - A_{12}A_{22}^{-1}A_{21}$, which turns out to be a positive definite symmetric matrix. Take vectors $\mathbf{a}_1, \ldots, \mathbf{a}_d \in \mathbb{R}^d$ such that $\Gamma = \big(\langle \mathbf{a}_i, \mathbf{a}_j \rangle\big)$, which is to be a $\mathbb{Z}$-basis of the Bravais lattice of the crystal $\Phi(X)$.

(3) Compute $\mathbf{b}(e) = {}^t\big(\langle e, \alpha_1\rangle, \ldots, \langle e, \alpha_b\rangle\big)$ $(e \in E_0)$, and $\mathbf{a}(e) = A^{-1}\mathbf{b}(e) = {}^t\big(a_1(e), \ldots, a_b(e)\big)$. Then putting $\mathbf{v}(e) = \sum_{i=1}^{d} a_i(e)\mathbf{a}_i$, we obtain a building block $\{\mathbf{v}(e)\}_{e\in E_0}$ of the canonical placement $\Phi : X \longrightarrow \mathbb{R}^d$.

Thus the most important part in the procedure is to take a $\mathbb{Z}$-basis of $H_1(X_0, \mathbb{Z})$ (preferably a $\mathbb{Z}$-basis represented by closed paths) with which everything reduces computation of matrices.

Remark 1 The canonical placement explained here is what we called the *standard realization* in [27] (2000), which derives from the asymptotic behaviors of random walks on topological crystals. Originally the standard realizations were introduced as an analogue of the Abel-Jacobi maps in algebraic geometry.

The reader may find a quite a bit analogy with the classical theory of *harmonic integrals* in the above discussion. Actually everything we explained here is a discrete version of the *method of orthogonal projections* developed by Weyl, Hodge, and Kodaira. A protoidea in the graph setting is already seen in Weyl's work in 1920s applied to the problem of electric circuits (see [39]).

Remark 2 Crystallographers also sought canonical ways to place periodic graphs in space, and proposed the notions of *archetype embeddings* (Eon [22], 1999), *archetypical representations* (Eon [23], 2011), *equilibrium placements* or *barycentric placements* (Delgado-Friedrichs and O'Keeffe [12], 2003), and *barycentric drawings* (Delgado-Friedrichs [14], 2004)[37].

The equilibrium placement coincides with the *harmonic realization* introduced in [27] (2000) as a special case of *harmonic maps* ([20], [31]), and hence is characterized as a minimizer of the energy functional with a fixed homomorphism ρ. Delgado-Friedrichs and O'Keeffe [12] rediscovered this fact. The first person in crystallography who seems to have mentioned the idea of equilibrium placements is H-J. Klein [26] (1996). The archetype embeddings introduced by Eon is a special equilibrium placement of the maximal topological crystal (minimal net) which is constructed in the same way as Φ^{ab}. Actually, reading off the terminology in [23] (being not an easy task), one may find that the archetypical representations are identical to the canonical placements.

13. Examples

We are now ready to produce examples of canonical placements based on the general recipe given in the previous section. An interesting aspect is that "beautiful" shapes of various crystal structures are characterized by

[37] Delgado-Friedrichs constructed a poweful algorithm (called *SYSTRE*) for the barycentric drawing. The program is available at http://www.gavrog.org/. An input data for SYSTRE is a finite graph together with an initial building block (with values in $\mathbb{Z}^d$), whereas the input data of our algorithm is a finite graph and a vanishing group.

the minimal principle. This reminds us of the isoperimetric inequality which characterizes the round circle, the most symmetric closed curve.

(1) Figure 21 illustrates the canonical placements of the quadrangle lattice, hexagonal lattice, triangular lattice, and kagome lattice[38]. They are called the *square lattice* (**sq1**), *honeycomb lattice* (**hcb**) (or *regular hexagonal lattice*), *regular triangular lattice* (**hx1**), and *regular kagome lattice* (**kgm**), respectively. Taking a look at their building blocks, we can easily check that these placements are actually canonical.

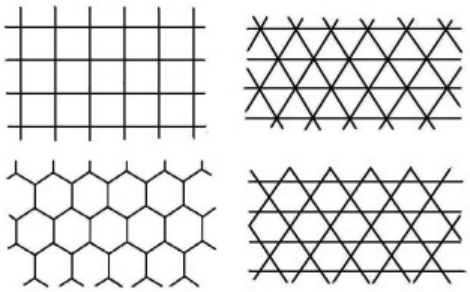

FIGURE 21. Classical 2-dimensional lattices

Here the regular kagome lattice is the canonical placement of the topological crystal over the graph depicted in Figure 22 with the vanishing group

$$H = \mathbb{Z}(e_1 + e_2 + e_3) + \mathbb{Z}(f_1 + f_2 + f_3).$$

It is known that some minerals, for instance jarosites ($KFe^{3+}{}_3(OH)_6(SO_4)_2$) and herbertsmithite ($ZnCu_3(OH)_6Cl_2$), contain layers with kagome lattice arrangement of atoms in their crystal structure.

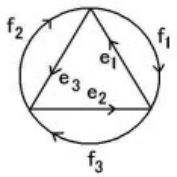

FIGURE 22. A fundamental finite graph of the kagome lattice

Figure 23 is a tiling of pentagons with picturesque properties that has become known as the *Cairo pentagon*[39]. Its 1-skeleton is the canonical placement of a topological crystal over the finite graph depicted on the right.

Figure 24 is the canonical placement associated with the *rhombille tiling* (**kdg**) which has an action by translations of the lattice group generated by two vectors (represented by arrows). The quotient graph is the one on the right.

[38]The term "kagome" derives from two separate Japanese words, meaning the pattern of holes ("me", literally "eyes") in a basket ("kago").

[39]This is also called Macmahon's net or **mcm**.

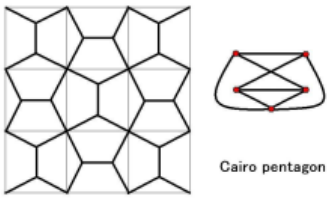

FIGURE 23. Cairo Pentagon

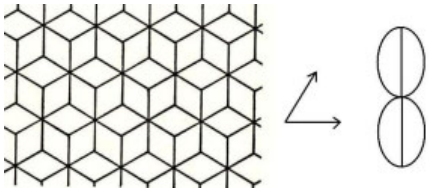

FIGURE 24. Dice pattern lattice

(2) Some of real crystals are canonically placed. Here are six examples:
(i) **Diamond** (**dia**)
(ii) **Lonsdaleite** (**lon**)
(iii) **Cubic lattice** (**pcu**)
(vi) **Face-centered cubic lattice** (**fcu**)
(v) **Body-centered cubic lattice** (**bcu**)
(vi) **3D kagome lattice** (**crs**)

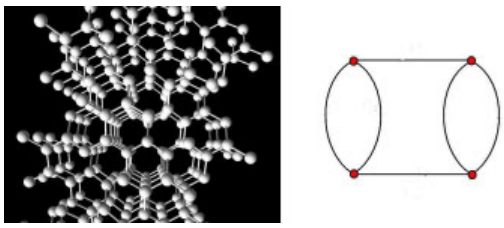

FIGURE 25. $ThSi_2$ structure

$ThSi_2$ structure. Figure 25 is the canonical placement of what crystallographers call the $ThSi_2$ structure, which is realized in a compound of Thorium and Silicide, and found in a number of other materials. As an abstract graph, $ThSi_2$ structure is the maximal topological crystal over the finite graph depicted on the right.

(3) We shall exhibit several hypothetical crystals.

(i) The K_4 crystal is the canonical placement of the maximal topological crystal over the complete graph K_4 ([38]).

The K_4 crystal is a purely mathematical object at present, not having been known so far to exist in nature as a pure crystal like diamond, but

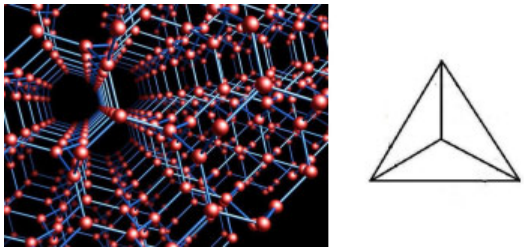

FIGURE 26. CG image of the K_4 crystal

possessing remarkable mathematical properties by which the K_4 crystal deserves to be called the *diamond twin* (see Section 14 and [38]).

The K_4 crystal, which I rediscovered by chance in the midst of my study of random walks, is called $(\mathbf{10},\mathbf{3})$-**a** ([42]) or **srs** net ([13]) by crystallographers (for more on the history of **srs** see [25]). The name **srs** comes from the fact that it occurs in the compound $SrSi_2$ as the Si substructure. H. S. M. Coxeter [10] called it "Laves' graph of girth ten". It is believed that the crystallographer who discovered for the first time this crystal structure as a hypothetical crystal is Fritz H. Laves (1933). The K_4 crystal has a close relationship with the gyroid, an infinitely connected triply periodic minimal surface discovered by Alan Schoen in 1970. In [9], the K_4 crystal is called the *triamond net*.

(ii) (**tfa**) Figure 27 is the canonical placement of the maximal topological crystal over the graph depicted on the right.

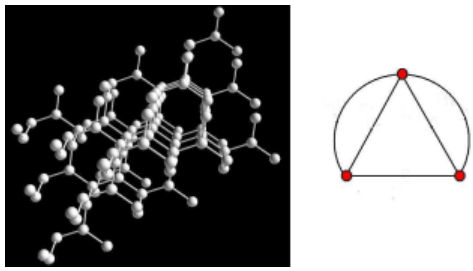

FIGURE 27. 3D example

(iii) Figure 28 is the canonical placement of the topological crystal over the graph depicted on the right (called K_{33}) corresponding to the vanishing subgroup $H = \mathbb{Z}(e_1 + e_2 + e_3 + e_4 + e_5 + e_6)$.

(iv) **3D kagome lattice** depicted in Figure 14 is usually regarded as a 3D analogue of the kagome lattice in crystallography since the 2D kagome lattice is a network of corner-sharing triangles while 3D kagome lattice is comprised of corner-sharing tetrahedra.

There is another 3D analogue of the kagome lattice which is defined to be the canonical placement of the topological crystal over the graph depicted

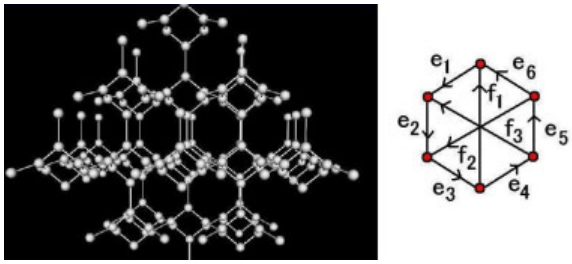

FIGURE 28. 3D example

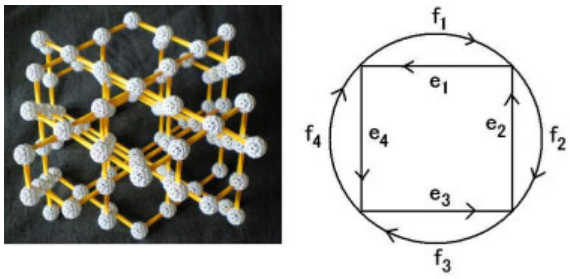

FIGURE 29. Another 3D kagome lattice

on the right in Figure 29 with the vanishing subgroup

$$H = \mathbb{Z}(e_1 + e_2 + e_3 + e_4) + \mathbb{Z}(f_1 + f_2 + f_3 + f_4)$$

(compare with the description of the kagome lattice given in (1)).

(v) The case that X_0 is the graph depicted on the right in Figure 30 with the vanishing subgroup

$$H = \mathbb{Z}(e_1 + e_2 + e_3 + e_4) + \mathbb{Z}(f_1 + f_2 + f_3 + f_4).$$

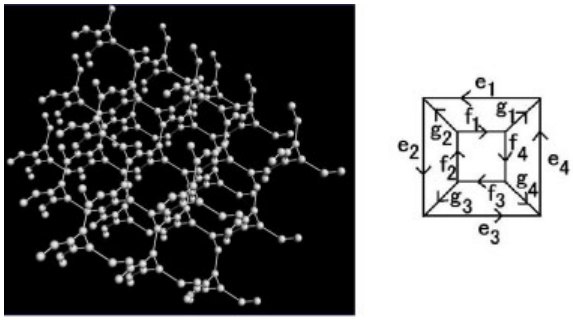

FIGURE 30. 3D example

14. Open problems

As mentioned in Section 2, the curiosity of Greek mathematicians about the beautiful shapes led to the classification of regular convex polyhedra.

This is also the case of Kepler who established the complete classification of semi-regular polyhedra. Namely an eager desire to explore beautiful forms has been the pulling force in geometry.

The open problems proposed here are concerned with the classification of crystal structures with big symmetry. We are thus following the long tradition of geometry[40].

An *isotropic*[41] crystal is a crystal with the property that there is no distinction in any direction and position in the sense that there is a congruent transformation preserving the crystal and exchanging any two directed edges. An isotropic crystal as an abstract graph has constant degree.

In the 2-dimensional case, such crystals are the classical lattices mentioned at the beginning of the previous section; that is,

(i) Square lattice,
(ii) Honeycomb lattice,
(iii) Regular triangular lattice,
(iv) Regular kagome lattice,

together with three series of pathological crystals (see Figure 31 for an example of isotropic pathological 2D crystal[42]).

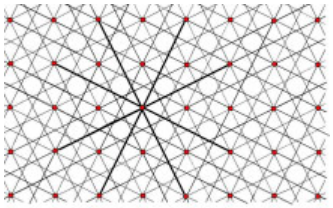

FIGURE 31. A pathological isotropic crystal

Here are (non-pathological) 3D examples known heretofore:

(i) K_4 crystal,	degree 3
(ii) Diamond,	degree 4
(iii) 3D kagome lattice (in our sense),	degree 4
(iv) Cubic lattice,	degree 6

[40]Here we take for granted the belief that beauty is bound up with symmetry. However human's aesthetic sense is not so simple to take the belief above as a complete agreement. Someone says cynically that "symmetry is death" since, if something has symmetry, it is static, unchanging, frozen as in death. Needless to say, aesthetic sense depends heavily upon our cultural background. For instance, compare the asymmetric feature of Japanese architecture with the so-called Greco-Roman tradition that strictly obeys the rule of symmetry.

[41]The term "isotropic" is used in a different context in crystallography. That is, an isotropic crystal is a crystal which has the same optical properties in all directions.

[42]This figure is placed in my book [37] published in 2006, and is called a *Pythahorian lattice* because it is related to rational solutions of the equation $x^2 + y^2 = 1$. See [19] (2009) (and [17], [18]) for a related question in which a weaker version (*edge-transitivity*) of isotropy is discussed.

(v) 3D kagome lattice, degree 6
(vi) Body-centered cubic lattice, degree 8
(vii) Face-centered cubic lattice, degree 12

Problem 1 Classify all 3D isotropic crystals including pathological ones[43].

One can consider a stronger version of isotropy. An isotropic crystal is said to be *strongly isotropic* if, for any two edges with the same end point, there is a congruent transformation preserving the crystal and exchanging these two edges while other edges (with the same end point) are fixed.

The K_4 and diamond crystals are the only two 3D crystals having the strong isotropic property (this is the reason why we call the K_4 crystal the diamond twin). In two dimension, the honeycomb lattice is the only example. A typical example in $\mathbb{R}^d$ is the d-dimensional diamond, the canonical placement of the maximal topological crystal over the graph consisting of 2 vertices joined by $d+1$ parallel edges. The maximal topological crystal over the complete graph K_n also yields an example, whose dimension is $(n-1)(n-2)/2$. Besides the 4-dimensional diamond, the maximal topological crystal over the graph in Figure 28 gives a 4D example.

Problem 2 Classify all strongly isotropic crystals of general dimension.

15. Discrete Abel-Jacobi maps

The canonical placement Φ^{ab} of the maximal topological crystal X_0^{ab} constructed in Section 12 has a special feature, which is properly interpreted by analogy with classical algebraic geometry. The reader may usefully consult the reference [2], [3], [6], [29], [39] for more about "discrete algebraic geometry", an active field still in a state of flux.

For the convenience of the reader, we shall start with a brief review of a relevant part in classical algebraic geometry.

Given an algebraic curve[44] S with a reference point p_0, we denote by $\Omega^1(S)$ the space of holomorphic 1-forms on S, and think of the first homology group $H_1(S,\mathbb{Z})$ as a subgroup of the dual space $\big(\Omega^1(S)\big)^*$ by using the pairing map

$$([\alpha],\omega)=\int_\alpha \omega,$$

where $[\alpha]$ stands for the homology class of a 1-cycle α. Since $H_1(S,\mathbb{Z})$ is a lattice group of $\big(\Omega^1(S)\big)^*$, the factor group

$$J(S)=\big(\Omega^1(S)\big)^*/H_1(S,\mathbb{Z}).$$

[43]This problem is interesting in view of architectural design.

[44]Precisely speaking, we are considering a non-singular complex projective algebraic curve, or equivalently a closed Riemann surfarce.

is a complex torus, which we call *Jacobian* (torus). The *Albanese map* $\Phi : S \longrightarrow J(S)$ is the holomorphic map defined by the pairing

$$(\Phi(p), \omega) \equiv \int_{p_0}^{p} \omega \pmod{H_1(S, \mathbb{Z})}. \tag{7}$$

On the other hand, the *Picard group* is defined as the factor group

$$\mathrm{Pic}(S) = \mathrm{Div}^0(S)/\mathrm{Prin}(S),$$

where $\mathrm{Div}^0(S)$ is the group of divisors with degree 0, namely

$$\mathrm{Div}^0(S) = \Big\{ \sum_{p \in S} a_p p \in C_0(S, \mathbb{Z}) | \ \sum_{p \in S} a_p = 0 \Big\},$$

and $\mathrm{Prin}(S)$ is the group of principal divisors, which is defined to be the subgroup of $\mathrm{Div}^0(S)$ consisting of divisors

$$\sum_{p \in S} \mathrm{ord}_p(f) p. \tag{8}$$

associated with meromorphic functions f on S. Here $\mathrm{ord}_p(f)$ is the order of a pole or zero of f. A classical result in complex analysis tells $\sum_{p \in S} \mathrm{ord}_p(f) = 0$, and hence the divisor (8) belongs to $\mathrm{Div}^0(S)$.

The *Abel-Jacobi map* $\Psi : S \longrightarrow \mathrm{Pic}(S)$ is a holomorphic map defined by

$$\Psi(p) \equiv p - p_0 \qquad (\mathrm{mod}\ \mathrm{Prin}(S)).$$

Abel's theorem, one of the culmination of classical algebraic geometry, asserts that the correspondence $p - p_0 \mapsto \Phi(p)$ yields an isomorphism of $\mathrm{Pic}(S)$ onto $J(S)$. Thus under the identification between $\mathrm{Pic}(S)$ and $J(S)$, the Abel-Jacobi map coincides with the Albanese map.

Having the above review in mind, we are now going to deal with an analogue of Jacobian torus in discrete set-up. Let $X_0 = (V_0, E_0)$ be a finite graph with a reference point x_0. Define the flat torus $J(X_0)$ by setting

$$J(X_0) = H_1(X_0, \mathbb{R})/H_1(X_0, \mathbb{Z}),$$

where the flat metric is the one induced from the inner product introduced in Section 12. We call $J(X_0)$ the *Jacobian torus*[45], which has the structure of abelian group at the same time.

Now let $\Phi^{\mathrm{ab}} : X_0^{\mathrm{ab}} = (V^{\mathrm{ab}}, E^{\mathrm{ab}}) \longrightarrow H_1(X_0, \mathbb{R})$ be the canonical placement of X_0^{ab} with $\Phi^{\mathrm{ab}}(x_0) = \mathbf{0}$. Since

$$\Phi^{\mathrm{ab}}(\alpha x) = \Phi^{\mathrm{ab}}(x) + \alpha \qquad (\alpha \in H_1(X_0, \mathbb{Z})),$$

we obtain a piecewise linear map $\Phi_0^{\mathrm{ab}} : X_0 \longrightarrow J(X_0)$. This is what we regard as an analogue of Albanese map.

[45]This is also called the Albanese torus.

To see a resemblance between a holomorphic Albanese map and its graph-theoretic analogue, we introduce the notion of *harmonic* 1-*form*[46] as an analogue of holomorphic 1-form. A harmonic 1-form on X_0 is defined to be a function $\omega : E_0 \longrightarrow \mathbb{R}$ satisfying

$$\omega(\overline{e}) = -\omega(e) \qquad (e \in E_0), \tag{9}$$

$$\sum_{e \in E_{0x}} \omega(e) = 0 \qquad (x \in V_0). \tag{10}$$

Then

$$(\Phi_0^{\mathrm{ab}}(x), \omega) \equiv \omega(e_1) + \cdots + \omega(e_n) \quad \big(\mathrm{mod}\ H_1(X_0, \mathbb{Z})\big) \tag{11}$$

for every harmonic 1-form ω and $x \in V_0$, where $(e_1, \ldots, e_n)$ is a path in X_0 joining x_0 and x. The pairing on the left hand side is defined by

$$\Big(\sum_{e \in E_0} a_e e, \omega \Big) = \sum_{e \in E_0} a_e \omega(e).$$

The right hand side of (11) is regarded as an analogue of line integral along a curve.

To go further, we introduce the notion of *discrete Jacobian*, a direct discrete analogue of Jacobian in algebraic geometry.

The homology group $H_1(X_0, \mathbb{Z})$ with integral coefficients is an *integral lattice* in $H_1(X_0, \mathbb{R})$ in the sense that $\langle \alpha, \beta \rangle \in \mathbb{Z}$ for every $\alpha, \beta \in H_1(X_0, \mathbb{Z})$. Denote by $H_1(X_0, \mathbb{Z})^{\#}$ the *dual lattice* of $H_1(X_0, \mathbb{Z})$ in $H_1(X_0, \mathbb{R})$; that is,

$$H_1(X_0, \mathbb{Z})^{\#} = \{\alpha \in H_1(X_0, \mathbb{R}) |\ \langle \alpha, \beta \rangle \in \mathbb{Z} \text{ for every } \beta \in H_1(X_0, \mathbb{Z})\}.$$

Since the lattice $H_1(X_0, \mathbb{Z})$ is integral, we have $H_1(X_0, \mathbb{Z}) \subset H_1(X_0, \mathbb{Z})^{\#}$. Then the *discrete Jacobian* $\mathcal{J}(X_0)$ is defined to be the factor group

$$H_1(X_0, \mathbb{Z})^{\#} / H_1(X_0, \mathbb{Z}),$$

which is identified with a finite subgroup of the Jacobian torus $J(X_0)$.

Now we shall observe $\Phi_0^{\mathrm{ab}}(V_0) \subset \mathcal{J}(X_0)$. For any $e \in E_0$ and $\alpha \in H_1(X_0, \mathbb{Z})$, we find $\langle P_{\mathrm{ab}}(e), \alpha \rangle = \langle e, P_{\mathrm{ab}}(\alpha) \rangle = \langle e, \alpha \rangle \in \mathbb{Z}$, and $\mathbf{v}_{\mathrm{ab}}(e) = P_{\mathrm{ab}}(e) \in H_1(X_0, \mathbb{Z})^{\#}$. Therefore $\Phi^{\mathrm{ab}}(x) \in H_1(X_0, \mathbb{Z})^{\#}$ for every $x \in V_0^{\mathrm{ab}}$, which immediately leads to $\Phi_0^{\mathrm{ab}}(V_0) \subset \mathcal{J}(X_0)$.

We shall call the restriction $\Phi_0^{\mathrm{ab}} | V_0 : V_0 \longrightarrow \mathcal{J}(X_0)$ the *discrete Albanese map*.

Theorem 15.1. (1) $\Phi_0^{\mathrm{ab}}(V_0)$ *generates* $\mathcal{J}(X_0)$.

(2) *The order* $|\mathcal{J}(X_0)|$ *coincides with the number of spanning trees* $\kappa(X_0)$ *in* X_0.

The proof of (1) is carried out as follows. Take a spanning tree T of X_0, and let $e_1, \ldots, e_b, \overline{e_1}, \ldots, \overline{e_b}$ $(b = b_1(X_0))$ be all edges not in T. Then $\mathbf{v}_{\mathrm{ab}}(e_1), \ldots, \mathbf{v}_{\mathrm{ab}}(e_b)$ constitute a $\mathbb{Z}$-basis of $H_1(X_0, \mathbb{Z})^{\#}$. This is because

[46]The notion of harmonic forms is originally introduced in Riemannian geometry. It is related to *cohomology theory* of manifolds.

we may take a $\mathbb{Z}$-basis of $H_1(X_0, \mathbb{Z})$ consisting of circuits $c_1, \ldots, c_b$ in X_0 such that c_i contains e_i, and $\langle c_i, \mathbf{v}_{\mathrm{ab}}(e_j)\rangle = \langle c_i, P_{\mathrm{ab}}(e_j)\rangle = \langle P_{\mathrm{ab}}(c_i), e_j\rangle = \langle c_i, e_j\rangle = \delta_{ij}$ (namely $\{\mathbf{v}_{\mathrm{ab}}(e_1), \ldots, \mathbf{v}_{\mathrm{ab}}(e_b)\}$ is the dual basis of $\{c_1, \ldots, c_b\}$). From this fact, our assertion immediately follows.

See [29] for the proof of (2).

The discrete Jacobian $\mathcal{J}(X_0)$ has a natural graph structure defined as follows. Let E_0^o be an orientation of X_0. The proof of Theorem 15.1 tells that $\{\mathbf{v}_{\mathrm{ab}}(e)\}_{e\in E_0^o}$ generates $\mathcal{J}(X_0)$. Thus the map $i : E_0^o \longrightarrow \mathcal{J}(X_0)$ defined by

$$i(e) = \mathbf{v}_{\mathrm{ab}}(e) \bmod H_1(X_0, \mathbb{Z}),$$

yields a connected graph $X\big(\mathcal{J}(X_0), E_0^o\big)$; that is, the Cayley-Serre graph associated with the map i (see the remark below), which we denote by $\mathcal{J}(X_0)$ by abuse of language. It is easy to see that the graph structure does not depend upon the choice of an orientation. If we assign the edge $\big(\Phi_0^{\mathrm{ab}}\big(o(e)\big), e\big)$ of $\mathcal{J}(X_0)$ to each $e \in E_0^o$, then, forgetting the orientation, we get a morphism $\Phi_0^{\mathrm{ab}} : X_0 \longrightarrow \mathcal{J}(X_0)$.

Remark Let G be a group, and $i : A \longrightarrow G$ be a map of a finite set A into G such that $i(A)$ generates G. We define the *Cayley-Serre graph* $X(G, A)$ in the following way (cf. [36]). The set V of vertices is just G. Directed edges are the pairs $(g, a),\ g \in G,\ a \in A$. The origin and terminus of the edge (g, a) are defined to be g and $gi(a)$, respectively. Forgetting orientation, we get a connected regular graph $X(G, A)$ of degree $2|A|$. The graph $X(G, A)$ has a natural free G-action given by $g(g', a) = (gg', a)$. Thus given a subgroup H of G, one can consider the quotient graph $X(G, A)/H$, called the *Schreier graph*, whose vertices are right cosets of H. In particular, $X(G, A)/G$ is the $|A|$-bouquet graph. In other words, the Cayley-Serre graph $X(G, A)$ is a regular covering graph over a bouquet graph.

Conversely, a regular covering graph over a bouquet graph is identified with a Cayley-Serre graph.

We define the *group of divisors of degree zero* in the discrete category by setting

$$\mathrm{Div}^0(X_0) = \Big\{ \sum_{x\in V_0} a_x x \in C_0(X_0, \mathbb{Z}) \big|\ \sum_{x\in V_0} a_x = 0 \Big\},$$

and the *group of principal divisors* by

$$\mathrm{Prin}(X_0) = (\partial \circ \partial^*)\big(C_0(X_0, \mathbb{Z})\big),$$

where ∂^* is the ajoint of ∂. Obviously $\mathrm{Prin}(X_0)$ is a subgroup of $\mathrm{Div}^0(X_0)$. Define the *discrete Picard group* by

$$\mathrm{Pic}(X_0) = \mathrm{Div}^0(X_0)/\mathrm{Prin}(X_0).$$

The order $|\mathrm{Pic}(X_0)|$ turns out to be equal to $\kappa(X_0)$.

Now we are ready to introduce a discrete version of Abel-Jacobi map. Imitating the case of algebraic curves, we define the *discrete Abel-Jacobi*

map $\Phi_0^{\mathrm{aj}} : V_0 \longrightarrow \mathrm{Pic}(X_0)$ by

$$\Phi_0^{\mathrm{aj}}(x) \equiv x - x_0 \qquad (\mathrm{mod}\ \mathrm{Prin}(X_0)).$$

An important fact is that the discrete Abel-Jacobi map has the following "universal" property (cf. [3]).

Theorem 15.2. *Let A be an additive group. Given a harmonic function $f : V_0 \longrightarrow A$ with $f(x_0) = 0$, there exists a unique homomorphism $\psi : \mathrm{Pic}(X_0) \longrightarrow A$ such that $\psi \circ \Phi_0^{\mathrm{aj}} = f$.*

In the above, a function $f : V_0 \longrightarrow A$ with values in A is said to be *harmonic* if

$$\sum_{e \in E_{0x}} \big[f\big(t(e)\big) - f\big(o(e)\big) \big] = 0.$$

The discrete Albanese map is a harmonic function on V_0 with values in $\mathcal{J}(X_0)$.

The following theorem, a discrete analogue of Abel's theorem, tells that the discrete Abel-Jacobi map is essentially the same as the discrete Albanese map.

Theorem 15.3. (**A discrete version of Abel's theorem**) *There exists a unique isomorphism φ of* $\mathrm{Pic}(X_0)$ *onto $\mathcal{J}(X_0)$ such that $\varphi \circ \Phi_0^{\mathrm{aj}} = \Phi_0^{\mathrm{ab}}$.*

The proof goes as follows. Use the universal property of discrete Abel-Jacobi maps to find a unique homomorphism $\varphi : \mathrm{Pic}(X_0) \longrightarrow \mathcal{J}(X_0)$ satisfying $\varphi \circ \Phi_0^{\mathrm{aj}} = \Phi_0^{\mathrm{ab}}$. Since $\Phi_0^{\mathrm{ab}}(V_0)$ generates $\mathcal{J}(X_0)$, we conclude that φ is surjective. That φ is an isomorphism is a consequence of the fact $|\mathcal{J}(X_0)| = \kappa(X_0) = |\mathrm{Pic}(X_0)|$.

16. Appendix

For the convenience of the reader, we shall give a "dictionary" of terminology used in crystallography ([22]) and mathematics.

(i) Cycle space = homology group $H_1(X_0, \mathbb{R})$

(ii) Cocycle space = the orthogonal complement of $H_1(X_0, \mathbb{R})$ in the 1-chain group $C_1(X_0, \mathbb{R})$ with respect to the canonical inner product

(iii) Labelled (quotient) graph= a finite graph with a building block

(iv) Cyclomatic number= the first Betti number

(v) Minimal net = the maximal abelian covering graph

(vi) Edge space= 1-chain group $C_1(X_0, \mathbb{Z})$

(vii) Equilibrium placement = harmonic realization

(viii) Archetypical representation = standard realization (canonical placement)

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