On the K_4 crystal

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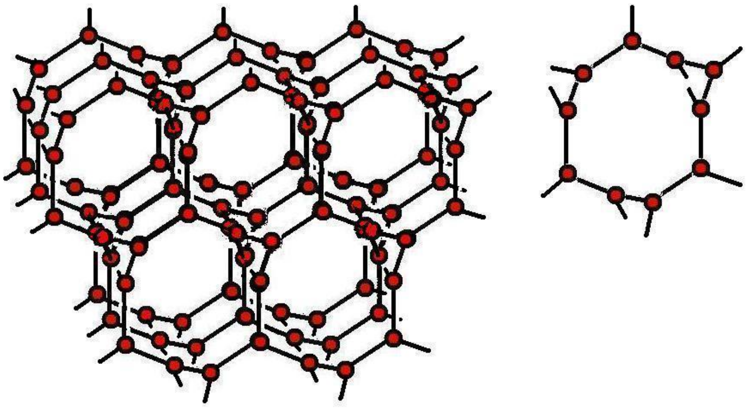
What's the K_4 crystal ?

The K_4 crystal is the most symmetric realization in $\mathbb{R}^3$ of the maximal abelian covering graph of the complete graph K_4.

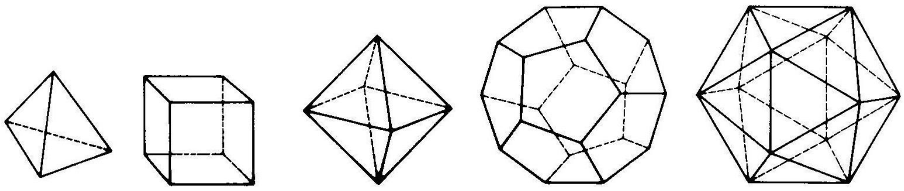


One can see a beautiful web of congruent decagonal rings.

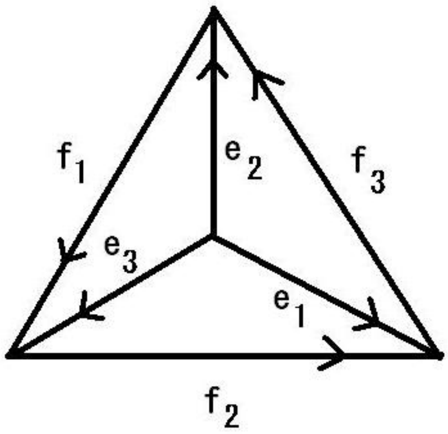
How special is this crystal ?

From the time of Greek mathematics, it is a typical nature of geometers to explore the feature of beautiful figures.

The classification of regular polyhedra



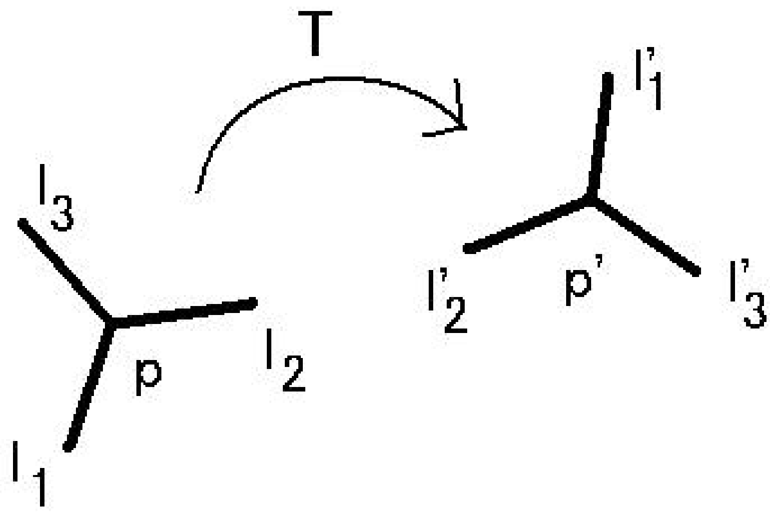
The complete graph K_4



K_n denotes the complete graph with n vertices.

Observations

- The K_4 crystal is a regular graph of degree 3.
- (very strong isotropic property) Let p and p' be vertices of the K_4 crystal. Let ℓ_1, ℓ_2, ℓ_3 be the edges with the end point p, and $\ell'_1, \ell'_2, \ell'_3$ be the edges with the end point p'. Then there exists a congruent transformation T leaving the K_4 crystal invariant such that $T(p) = p'$ and $T(\ell_i) = \ell'_i$ $(i = 1, 2, 3)$.


T
l'1
l3
l'2
p'
l'3
p
l2
l1

∘ (maximal symmetry) Let g be an arbitrary automorphism of the K_4 crystal as an abstract graph. Then one can find a congruent transformation T leaving the K_4 crystal invariant and giving rise to g.

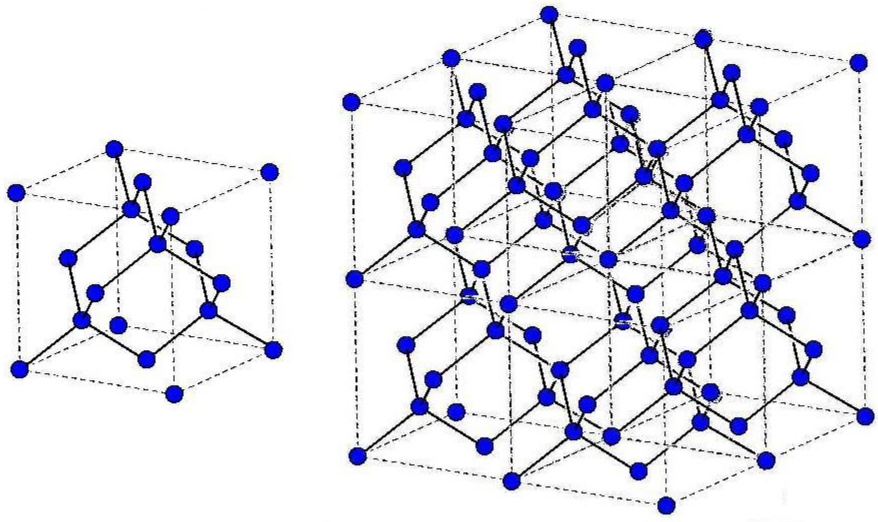
∘ (energy minimizing property) Among all crystals obtained as realizations of the maximal abelian covering graph of K_4, the K_4 crystal minimizes the energy.

There is another crystal in $\mathbb{R}^3$ having the similar properties

- **very strong isotropic property,**
- **maximal symmetry,**
- **energy minimizing property,**

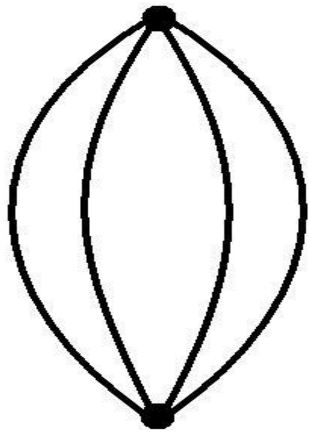
that is,

the diamond crystal



One can see a web of congruent hexagonal rings.

The diamond crystal is the most symmetric realization of the maximal abelian covering graph of the graph consisting of 2 vertices and 4 multiple edges joining them.



A big difference between the K_4 crystal and the diamond crystal

∘ **The K_4 crystal has chirality, that is, its mirror image can not be superposed on the original one by a rigid motion.**

∘ **The diamond crystal has no chirality.**

Main Theorem

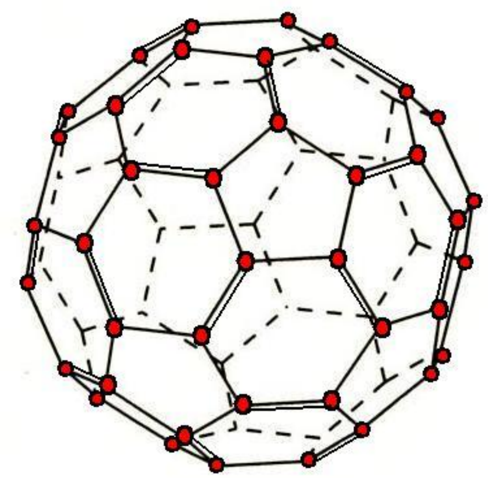
A crystal in $\mathbb{R}^3$ with very strong isotropic property and energy minimizing property is either the diamond crystal or the K_4 crystal (and its mirror image).

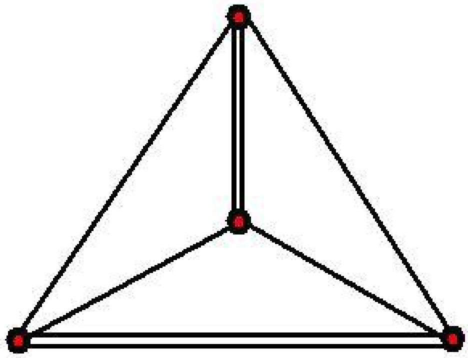
Non-mathematical problem: Does there exist the K_4 crystal in the real world ? More specifically, can carbon atoms form the K_4 crystal (allowing double bonds) ?

If exists, what about its physical nature ?

Fullerene C_{60}

The truncated icosahedron (one of Archimedean polyhedra) is realized as a compound of cabon atoms.





The lifting of these double bonds to the maximal abelian covering graph gives the K_4 crystal of valency 4.

Notations and conventions

◦ A graph is denoted as $X = (V, E)$, where

$$\begin{aligned} V &= \text{the set of vertices}, \\ E &= \text{the set of all oriented edges} \end{aligned}$$

$$\begin{aligned} o(e) &= \text{the origin of } e \in E, \\ t(e) &= \text{the terminus of } e \in E, \\ \bar{e} &= \text{the inversion of } e \in E. \end{aligned}$$

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

Definition

A graph $X = (V, E)$ is said to be a d-dimensional crystal lattice if Aut(X) has a free abelian subgroup Γ of rank d such that

(1) Γ acts freely both on V and the set of non-oriented edges, and

(2) the quotient graph $X_0 = \Gamma\backslash X$ is finite.

The group Γ is said to be a lattice (group) of X, and $X_0 = (V_0, E_0)$ is said to be the fundamental finite graph, where $V_0 = \Gamma\backslash V$, $E_0 = \Gamma\backslash E$.

∘ In other words, a crystal lattice is an abelian covering graph of a finite graph with a free abelian covering transformation group.

∘ This interpretation is useful for a systematic construction of crystal lattices. Actually, given a free abelian group Γ, a finite graph X_0 and a surjective homomorphism $\mu : H_1(X_0, \mathbb{Z}) \longrightarrow \Gamma$, we may construct a crystal lattice with the lattice group Γ and the fundamental finite graph X_0.

∘ The K_4 crystal as an abstract graph is called the K_4 lattice.

∘ The diamond crystal as an abstract graph is called the diamond lattice.

The maximal abelian covering graph

This is the case that

$$\Gamma = H_1(X_0, \mathbb{Z}),$$
$$\mu = \text{the identity map}$$

Example: The maximal abelian covering graph of the graph consisting of two vertices and 3 multiple edges joining them is the haxagonal lattice.

Definition

Let $X = (V, E)$ be a d-dimensional crystal lattice. A map $\Phi : V \longrightarrow \mathbb{R}^d$ is said to be a periodic realization of X if there exist a lattice group Γ and an injective homomorphism $\rho : \Gamma \longrightarrow \mathbb{R}^d$ such that

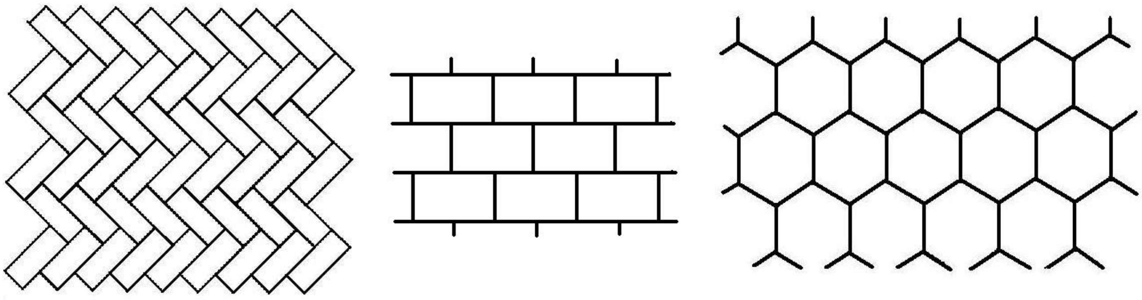
(1) $\Phi(gx) = \Phi(x) + \rho(g)$ for $x \in V$ and $g \in \Gamma$.

(2) $\rho(\Gamma)$ is a lattice in $\mathbb{R}^d$. Here a lattice means a discrete subgroup of $\mathbb{R}^d$ of maximal rank.

A crystal = a crystal lattice realized periodically in $\mathbb{R}^d$.

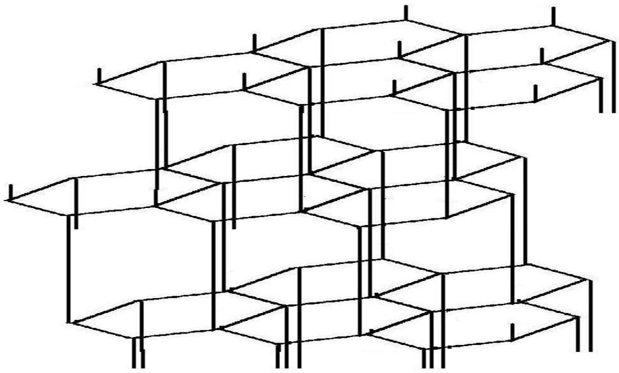
A crystal lattice has mamy periodic realizations !

Various periodic realizations of the hexagonal lattice



The most "standard" one is the realization of honeycomb type.

A periodic realization of the diamond lattice (of graphite type)



A building block for a crystal

A system of vectors $\{\mathrm{v}(e)\}_{e\in E_0}$ is defined by

$$\mathrm{v}(e) = \Phi\big(t(e)\big) - \Phi\big(o(e)\big) \quad (e \in E),$$

where we should note that the function v on E is invariant under the action of Γ so that it is regarded as a function on E_0. It is easily observed that $\{\mathrm{v}(e)\}_{e\in E_0}$ determines the periodic realization Φ. In this sense, $\{\mathrm{v}(e)\}_{e\in E_0}$ is called a building block.

A building block for the K_4 crystal

Take vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ in $\mathbb{R}^3$ satisfying $\|\mathbf{a}_1\|^2 = \|\mathbf{a}_2\|^2 = \|\mathbf{a}_3\|^2 = 3$, $\mathbf{a}_i \cdot \mathbf{a}_j = -1 \quad (i \neq j)$. Put

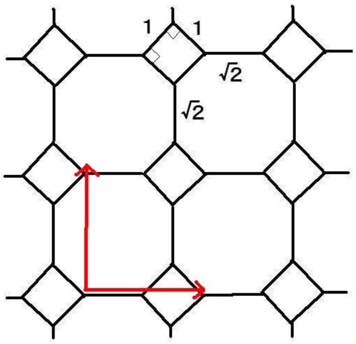
$$\begin{aligned}
&\mathbf{v}(e_1) = -\frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3, \quad \mathbf{v}(e_2) = \frac{1}{4}\mathbf{a}_1 - \frac{1}{4}\mathbf{a}_3, \\
&\mathbf{v}(e_3) = -\frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2, \\
&\mathbf{v}(f_1) = \frac{1}{2}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3, \quad \mathbf{v}(f_2) = \frac{1}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3, \\
&\mathbf{v}(f_3) = \frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3.
\end{aligned}$$

Then the vectors

$$\begin{gathered}
\pm\mathbf{v}(e_1), \pm\mathbf{v}(e_2), \pm\mathbf{v}(e_3), \\
\pm\mathbf{v}(f_1), \pm\mathbf{v}(f_2), \pm\mathbf{v}(f_3)
\end{gathered}$$

constitute the building block of the K_4 crystal.

To see that the K_4 crystal is actually a covering graph of K_4, we take a look at the K_4 crystal from some direction to observe that the K_4 crystal is a covering graph of the following 2-dimensional crystal.



We easily see that K_4 is the quotient graph of this graph by the translations group generated by two vectors depicted in the figure.

A periodic realization Φ is said to have maximal symmetry if there exists a homomorphism

$$\rho : \mathrm{Aut}(X) \longrightarrow M(d)$$

such that

$$\Phi(gx) = \rho(g)\Phi(x),$$

where $M(d)$ denotes the group of congruent transformations of $\mathbb{R}^d$.

Theorem

For every crystal lattice, there exists a periodic realization with maximal symmetry.

Among periodic realizations with maximal symmetry, there is a standard one, which is characterized as the energy minimizing realization.

Notations

$\boldsymbol{E_x}$ **denotes the set of oriented edges whose origin is** $\boldsymbol{x \in V}$

$\boldsymbol{d(x) = |E_x|}$ **denotes the degree of the vertex** $\boldsymbol{x}$

We shall define the energy of periodic realizations.

Energy

We define the energy of a crystal by regarding it as a system of harmonic oscillators.

Given a bounded domain $\mathfrak{D}$ in $\mathbb{R}^d$ and a periodic realization $\boldsymbol{\Phi}$, define $\mathfrak{E}_{\mathfrak{D}}(\boldsymbol{\Phi})$ by

$$\mathfrak{E}_{\mathfrak{D}}(\boldsymbol{\Phi}) = \frac{\mathcal{E}_{\mathfrak{D}}(\boldsymbol{\Phi})}{m_{\mathfrak{D}}(\boldsymbol{\Phi})^{1-2/d}\mathrm{vol}(\mathfrak{D})^{2/d}},$$

where

$$\mathcal{E}_{\mathfrak{D}}(\boldsymbol{\Phi}) = \frac{1}{2}\sum_{\substack{x\in V\\ \boldsymbol{\Phi}(x)\in\mathfrak{D}}}\sum_{e\in E_x}\|\mathrm{v}(e)\|^2,$$

$$m_{\mathfrak{D}}(\boldsymbol{\Phi}) = \sum_{\substack{x\in V\\ \boldsymbol{\Phi}(x)\in\mathfrak{D}}} d(x)$$

∘ **Roughly $\mathcal{E}_{\mathfrak{D}}(\boldsymbol{\Phi}) \sim \mathrm{vol}(\mathfrak{D})$, $\mathfrak{D}(\boldsymbol{\Phi}) \sim \mathrm{vol}(\mathfrak{D})$ as $\mathrm{vol}(\mathfrak{D}) \uparrow \infty$.**

∘ **For a homothetic transformation $\boldsymbol{T} = (\boldsymbol{\lambda A}, \mathrm{a})$,**

$$\begin{aligned}
&\mathcal{E}_{\mathfrak{D}}(\boldsymbol{T\Phi}) = \boldsymbol{\lambda}^2 \mathcal{E}_{\boldsymbol{T}^{-1}\mathfrak{D}}(\boldsymbol{\Phi}),\\
&\boldsymbol{m}_{\mathfrak{D}}(\boldsymbol{T\Phi}) = \boldsymbol{m}_{\boldsymbol{T}^{-1}\mathfrak{D}}(\boldsymbol{\Phi}),\\
&\mathrm{vol}(\mathfrak{D}) = \boldsymbol{\lambda}^d \mathrm{vol}(\boldsymbol{T}^{-1}\mathfrak{D}),
\end{aligned}$$

$$\text{thus } \mathfrak{E}_{\mathfrak{D}}(\boldsymbol{T\Phi}) = \mathfrak{E}_{\boldsymbol{T}^{-1}\mathfrak{D}}(\boldsymbol{\Phi}).$$

Take an increasing sequence of bounded domains $\{\mathfrak{D}_i\}_{i=1}^{\infty}$ with $\cup_{i=1}^{\infty}\mathfrak{D}_i = \mathbb{R}^d$ (for example, a family of concentric balls).

The energy is defined as the limit

$$\mathfrak{E}_0(\boldsymbol{\Phi}) = \lim_{i\to\infty} \mathfrak{E}_{\mathfrak{D}_i}(\boldsymbol{\Phi}).$$

∘ **The limit exists under a mild condition on $\{\mathfrak{D}_i\}_{i=1}^{\infty}$, and $\mathfrak{E}_0(\boldsymbol{\Phi})$ does not depend on the choice of $\{\mathfrak{D}_i\}_{i=1}^{\infty}$.**

- $\mathfrak{E}_0(T\Phi) = \mathfrak{E}_0(\Phi)$ **for any homothetic transformation** T**.**
- **If** Φ **is periodic with respect to a lattice group** Γ**, then**

$$\mathfrak{E}_0(\Phi) = \frac{\mathcal{E}(\Phi)}{m(X_0)^{1-2/d}\mathrm{vol}\big(\mathbb{R}^d/\rho(\Gamma)\big)^{2/d}},$$

where $m(X_0) = \sum_{x \in V_0} d(x) = |E_0|$**, and**

$$\mathcal{E}(\Phi) = \frac{1}{2}\sum_{e \in E_0} \|\mathrm{v}(e)\|^2.$$

Theorem

For a fixed crystal lattice X, the minimum of $\mathfrak{E}_0$ is attained by a periodic realization, which is unique up to homothetic transformations.

Energy minimizing periodic realization is said to be the standard realization.

∘ The standard realization is an analogue of Albanese maps in algebraic geometry.

Characterization of standard realizations

The standard realization Φ is characterized by

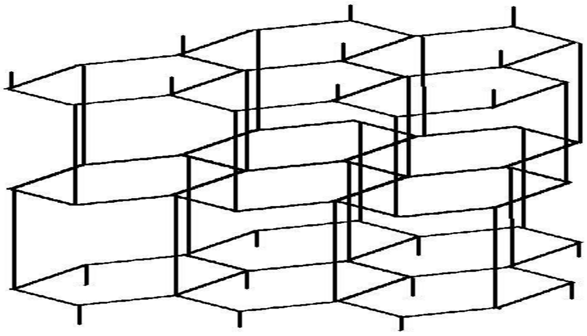
$$\sum_{e \in E_x} \mathrm{v}(e) = 0,$$
$$\sum_{e \in E_0} \big(\mathrm{x} \cdot \mathrm{v}(e)\big)^2 = c\|\mathrm{x}\|^2 \quad (\mathrm{x} \in \mathbb{R}^d),$$

(it is concluded that $c = \dfrac{2}{d}\mathcal{E}(\Phi)$)

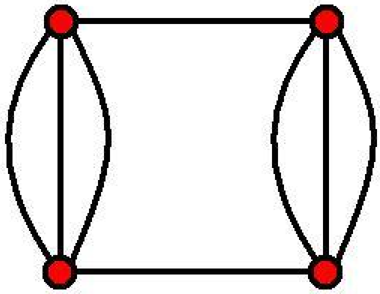
- **The K_4 crystal is the standard realization of the K_4 lattice.**
- **The diamond crystal is the standard realization of the diamond lattice.**

Lonsdaleit

Lonsdaleite is a rare stone of pure carbon and a kinsfolk of the diamond crystal, discovered at Meteor Crater, Arizona, in 1967, The great heat and stress of the impact caused when meteoric graphite falls to Earth is believed to form lonsdaleite. Lonsdaleite is also called hexagonal diamond.

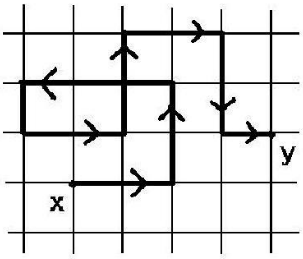


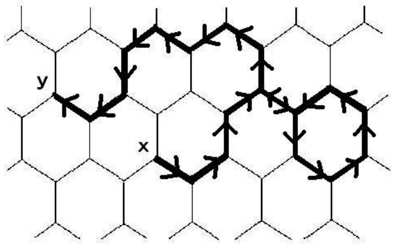
The Lonsdaleite crystal is the standard realization of an abelian covering graph of the following finite graph.



Facts behind the theorem

The standard realization has a close relation with asymptotic behavior of random walks on a crystal lattice.





Let $p(n, x, y)$ be the nth step transition probability for the simple randam walk on X.

Note that $p(n, x, y)$ is determined solely by the graph structure of X.

Relation between transition probabilities and standard realizations

There exists a positive constant C such that

$$C\|\Phi(x)-\Phi(y)\|^2 = \lim_{n\to\infty} 2n\Big\{\frac{p(n,x,x)}{p(n,y,x)} + \frac{p(n,y,y)}{p(n,x,y)} - 2\Big\}$$

∘ This is a consequence of the asymptotic expansion of $p(n,x,y)$ as n goes to infinity.

∘ This is used when we prove that the standard realization yields a realization with maximal symmetry.

Local limit formula: There exists a positive constant $C(X)$ such that

$$\lim_{n\to\infty}(4\pi n)^{d/2}p(n,x,y)d(y)^{-1} = C(X)$$

A geometric description of $C(X)$ was given by T. Shirai, M. Kotani and T. S.

X	hexagonal	triangular	quadrilateral	kagome
$C(X)$	$2\sqrt{3}$	$\frac{\sqrt{3}}{3}$	2	$\frac{2\sqrt{3}}{3}$

Theorem: For a fixed crystal lattice $\boldsymbol{X}$,

$$\min_{\boldsymbol{\Phi}} \mathfrak{E}_0(\boldsymbol{\Phi}) = \begin{cases} dC(X)^{-2/d} & \text{(non-bipartite case)} \\ d\left(\frac{C(X)}{2}\right)^{-2/d} & \text{(bipartite case)} \end{cases}$$

Open problem: Can the theorem above be generalized to a more general class of infinite graphs (for instance, quasi crystals) ?

Idea of the proof for the main thoerem

Let X be a crystal in $\mathbb{R}^3$ with very strong isotropic property and energy minimizing property.

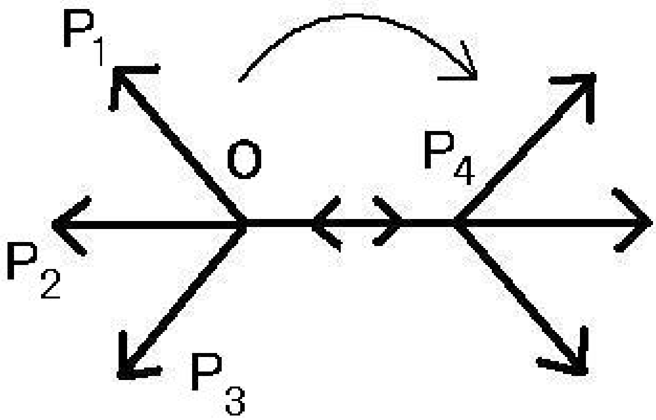
1. Show that the degree of X is 3 or 4.

More generally, for a d-dimensional very isotropic crystal lattice X, its degree n is less than or equal to $d+1$. To see this, consider $\mathrm{v}(e_1), \cdots, \mathrm{v}(e_n)$ ($e_i \in E_x$) for the standard realization. We then have $\sum_{i=1}^{n} \mathrm{v}(e_i) = 0$, and in view of the isotropy condition,

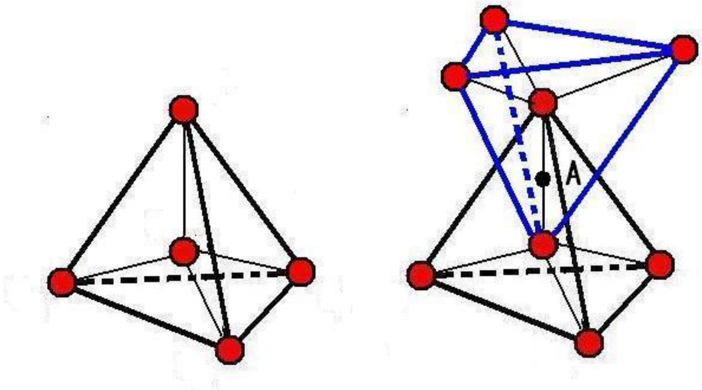
$$\|\mathrm{v}(e_i)\| \equiv a, \quad \mathrm{v}(e_i) \cdot \mathrm{v}(e_j) \equiv b \ (i \neq j),$$

from which it follows that $\mathrm{v}(e_1), \cdots, \mathrm{v}(e_{n-1})$ are linearly independent.

2. Consider the case of degree 4. For $\boldsymbol{e_1, e_2, e_3, e_4 \in E_x}$, the points $\boldsymbol{P_1, P_2, P_3, P_4}$ defined by $\boldsymbol{\overrightarrow{OP_i} = \mathrm{v}(e_i)}$ form the regular tetrahedron with the barycenter $\boldsymbol{O = \Phi(x)}$.



3. What we have to show is, in view of the structure of the diamond crystal, that for any edge $\boldsymbol{e}$, there exists $\boldsymbol{g} \in \mathbf{Aut}(\boldsymbol{X})$ such that $\boldsymbol{T}(\boldsymbol{g})$ is a point-symmetric transformation with respect to the midpoint of the segment $\boldsymbol{\Phi}(\boldsymbol{o}(\boldsymbol{e}))\boldsymbol{\Phi}(\boldsymbol{t}(\boldsymbol{e}))$.



4. Consider the case of degree 3. Use the fact that $\mathrm{Aut}(X)$ is a crystallographic group so that one has an exact sequence

$$0 \longrightarrow \Gamma \longrightarrow \mathrm{Aut}(X) \xrightarrow{p} K \longrightarrow 1,$$

where K is a finite subgroup of $O(3)$, and the lattice group Γ is the maximal abelian group of $\mathrm{Aut}(X)$.

5. Observe that K acts naturally on the fundamental finite graph X_0. It is enough to show that $|V_0| = 4$.

6. (the most difficult part) Show $K \subset SO(3)$.

7. Use the classification of finite subgroups of $SO(3)$:

(i) the cyclic group $\mathbb{Z}_n$

(ii) the dihedral group D_n

(iii) the tetrahedral group A_4

(iv) the octahedral group S_4

(v) the icosahedral group A_5

8. Note that the order of elements in K is $1, 2, 3, 4$, or 6 (a consequence of the fact that K leaves a lattice invariant) to conclude that $K = S_4$ and $|V_0| = 4$.

Problem

List all crystals in $\mathbb{R}^d$ with very strong isotropic property and energy minimizing property

∘ In the two dimensional case, the honeycomb is only one crystal satisfying these properties.

Two dimensional crystal satisfying weaker properties

A crystal lattice X is said to be (oriented) edge transitive if, for every $e_1, e_2 \in E$, there exists $g \in \mathrm{Aut}(X)$ such that $e_2 = ge_1$.

This property is strong enough to classify 2-dimensional (non-degenerate) crystal lattices.

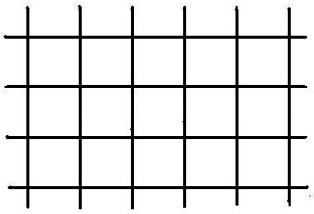
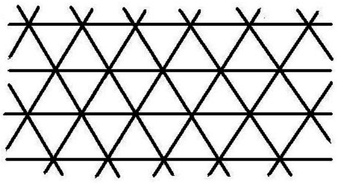
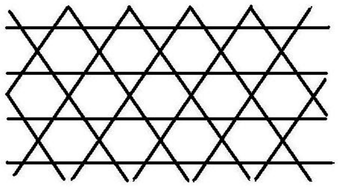
1. **Planar case**

    (a) **quadrilateral lattice**

    (b) **triangular lattice**

    (c) **hexagonal lattice**

    (d) **kagome lattice**

The figures above are the standard realizations of the quadrilateral lattice, triangular lattice, kagome lattice respectively.

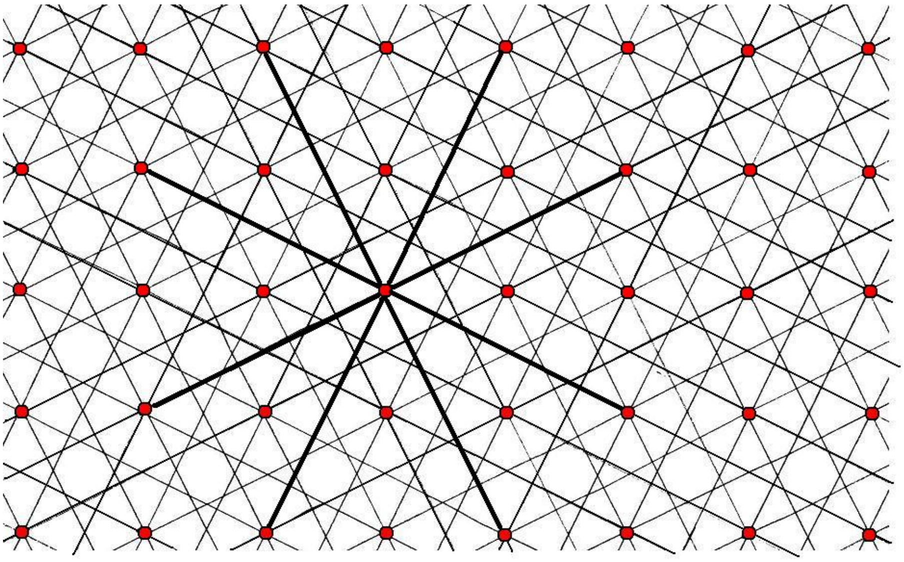
2. **Non-planar case**

   (a) **the crystal lattice constructed by merging the square lattice and its rotation with the angle θ determined by $\tan\theta = q/p$ where $(p, q) \in \mathbb{Q} \times \mathbb{Q}$, $p, q > 0$, $q/p \leq 1/2$, and $p^2 + q^2 = 1$**

   (b) **the crystal lattice constructed by merging the regular triangular lattice and its rotation with the angle θ determined by $\tan\theta = \sqrt{3}q/(2p - q)$ where $(p, q) \in \mathbb{Q} \times \mathbb{Q}$, $p, q > 0$, $q/(2p - q) \leq 1/3$, and $p^2 - pq + q^2 = 1$**

   (c) **the crystal lattice constructed by merging the hexagonal lattice and its rotation in the same way as above.**

Merging the square lattice and its rotation



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