

STANDARD REALIZATIONS OF CRYSTAL LATTICES VIA HARMONIC MAPS

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ABSTRACT. An Eells-Sampson type theorem for harmonic maps from a finite weighted graph is employed to characterize the equilibrium configurations of crystals. It is thus observed that the minimum principle frames symmetry of crystals.

1. INTRODUCTION

We shall start with the motivation behind the subject which we are concerned within this paper. A simplified model of *crystals* is a system of springs which connect masses distributed periodically in Euclidean space. The masses represent atoms, and the springs represent symbolically the internal forces binding two atoms in the crystal. A periodic structure of the system, which shows a peculiar feature of crystals, is described as invariance of the system under the action of an additive group of translations in the space. The smallest pattern unit of the crystal from which the whole crystal can be built up by translations is called a *primitive unit cell* of the system. The atoms in a real crystal are vibrating around their equilibrium positions with thermal motion. The atoms are supposed to rest at the equilibrium positions when the absolute temperature is zero.

The main problem considered in this paper is to find a geometric characterization for the *equilibrium configurations* of the atoms in the crystal. For instance, we ask why the crystal of diamond has such a beautiful configuration of the carbon atoms which assures the rigid structure of diamond (Figure 1 in §3).

This rather fundamental and simple question seems to have not yet been answered in full generality. The classical theory of crystallographic groups, a treatment of crystals from the viewpoint of symmetries and having a long history since 1830, does not give any satisfactory answer to the question. We have a macroscopic characterization of equilibrium shapes of crystals due to G. Wulff (1901), which also fails to give any microscopic characterization for configurations of the atoms in crystals.

An equilibrium configuration should satisfy the condition that the internal forces in the crystal are in equilibrium; that is, the total force acting on any atom from its nearest neighbors vanishes. This condition, however, is not enough to determine the equilibrium configuration uniquely. Actually, as is easily seen, the equilibrium of the internal forces is preserved by any affine transformation of the space.

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As a characterization of equilibrium configurations, we shall take up the “*minimum principle*” for the potential energy per primitive unit cell with a fixed volume, which seems natural from physical and mathematical points of view. Indeed, we establish the following theorem.

Theorem 1. *Among configurations of a given crystal having a primitive unit cell with a fixed volume, there exists a configuration with the minimal potential energy per primitive unit cell, and it is uniquely determined up to motions of the space.*

The proof of the above theorem is effectively reduced to the theory of *harmonic maps* from finite *weighted graphs* into *flat tori*, as will be explained in §3. In fact, we shall prove the following theorem which is regarded as a geometric version of the statement in Theorem 1.

Theorem 2. *Let X_0 be a finite connected weighted graph, \mathcal{T} a torus, and C a homotopy class of piecewise smooth maps from X_0 into \mathcal{T} such that a map in C induces the surjective homomorphism of $\pi_1(X_0)$ onto $\pi_1(\mathcal{T})$. For a given positive constant v_0 , there exists a pair (Φ_0, g_0) , consisting of a harmonic map $\Phi_0 \in C$ and a flat metric g_0 on \mathcal{T} such that $\text{vol}(\mathcal{T}, g_0) = v_0$, satisfying*

$$(1) \quad E(\Phi_0, g_0) \leq E(\Phi, g)$$

for every $\Phi \in C$ and every flat metric g on \mathcal{T} with $\text{vol}(\mathcal{T}, g) = v_0$, where $E(\Phi, g)$ denotes the energy of the map $\Phi : X_0 \rightarrow (\mathcal{T}, g)$. The pair (Φ_0, g_0) is determined uniquely. More precisely, if $E(\Phi, g) = E(\Phi_0, g_0)$, then $g = g_0$ and Φ coincides with a translation of Φ_0 .

The terminology used in the above theorem will be introduced in §2. In §4, we characterize the pair (Φ_0, g_0) in terms of a graph-theoretical analogue of the Albanese maps into Albanese tori, a concept originally introduced in algebraic geometry, and give a standard way to realize the configuration of the crystal satisfying the minimum principle.

As will be seen in §5, the classical configurations for many crystals in two and three dimension turn out to satisfy the minimum principle. The diamond crystal illustrates this characterization.

It should be pointed out that one may establish an analogue of Theorem 2 for harmonic maps from a compact Riemannian manifold into a flat torus.

Let us conclude this introduction by mentioning an unexpected relation of the standard realization of a crystal lattice X to the asymptotic behavior of the transition probability of a random walk on X (see [8] for the details).

Theorem. *Consider a reversible random walk on a crystal lattice X with an invariant measure m . We equip X with a canonical weighted structure. Let $d(x, y)$ be the distance on X induced from the Euclidean distance by the standard realization of X in \mathbb{R}^k . If X is not bipartite, then there exist positive constants C_1, C_2 such that, for the n -step transition probability $p(n, x, y)$,*

$$\lim_{n \uparrow \infty} \left[(4\pi n)^{k/2} p(n, x, y) m(y)^{-1} - C_1 \exp\left(-\frac{C_2}{n} d(x, y)^2\right) \right] = 0$$

uniformly for all $x, y \in X$.

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2. HARMONIC MAPS OF A WEIGHTED GRAPH INTO A RIEMANNIAN MANIFOLD

The notion of harmonic maps was introduced by J. Eells and J.H. Sampson in 1964 in their fundamental paper [2] as a generalization of geodesics, harmonic functions and holomorphic mappings between Kähler manifolds. As in the case of ordinary harmonic maps of Riemannian manifolds, harmonic maps of a finite weighted graph X into a Riemannian manifold Y are defined to be critical maps for the *energy functional* E , where the graph X is regarded as a 1-dimensional singular space, or precisely speaking, a 1-dimensional CW-complex, and maps are always supposed to be piecewise smooth. We shall explain these notions in detail.

Let $X = (V, E)$ be a connected locally finite graph with a set V of vertices and a set E of all oriented edges. For an edge $e \in E$, we denote by $o(e)$ and $t(e)$ the *origin* and the *terminus* of e respectively. The *inverse* edge of e will be denoted by \bar{e} . Consider positive valued functions m_V on V and m_E on E , where it is assumed that $m_E(\bar{e}) = m_E(e)$ for every $e \in E$. The functions m_V and m_E are said to be *weight functions* on V and E respectively. A graph with weight functions is called a *weighted graph*.

We first fix a way to identify the graph X with a CW-complex. Take the disjoint union $V \amalg (E \times [0, 1])$ and introduce the equivalence relation \sim defined by

$$(2) \quad \begin{aligned} o(e) &\sim (e, 0), \\ t(e) &\sim (e, 1), \\ (e, t) &\sim (\bar{e}, 1 - t) \text{ for } 0 \leq t \leq 1. \end{aligned}$$

Then the CW-complex associated with the graph X is defined as the quotient space $V \amalg (E \times [0, 1]) / \sim$ so that the unoriented edges (resp. vertices) are identified with 1-cells (resp. 0-cells). The CW-complex X is considered as a one-dimensional singular Riemannian manifold with the metric $ds^2 = m_E^2(e) dt^2$ on each edge $e \in E$.

Given a map Φ of X into a Riemannian manifold (Y, g) , we put $\Phi_e(t) = \Phi(e, t)$ for $e \in E$ and $0 \leq t \leq 1$; this is considered as the restriction of Φ to the edge e . The map Φ is said to be *piecewise smooth* if Φ is continuous and the curve Φ_e is smooth in t for every $e \in E$.

For a piecewise smooth map Φ of a finite weighted graph X into (Y, g) , define the *energy* of Φ by

$$(3) \quad E(\Phi) = E(\Phi, g) = \frac{1}{2} \sum_{e \in E} m_E(e) \int_0^1 \left\| \frac{d\Phi_e}{dt} \right\|^2 dt.$$

We shall compute the first and the second variation formulae. Let $\Phi(u, \cdot)$ ($|u| < \varepsilon$) be a smooth variation of a map $\Phi = \Phi(0, \cdot)$, and put

$$(4) \quad \frac{d\Phi_e}{dt} = \dot{\Phi}_e, \quad \frac{\partial \Phi_e}{\partial u}(u, t) = W_e(t), \quad \frac{\partial \Phi_e}{\partial u}(u, 0) = W(x),$$

where we abuse the notation and write $\Phi_e = \Phi_e(u, t)$.

Theorem 2.1 (The first and second variation formulae). *At $u = 0$, we have*

$$\begin{aligned}
(5) \quad \frac{dE(\Phi)}{du} &= -2 \sum_{x \in V} \langle W(x), \sum_{e \in E_x} m_E(e) \dot{\Phi}_e(0) \rangle \\
&\quad - \sum_{e \in E} m_E(e) \int_0^1 \langle W_e(t), \frac{D}{dt} \dot{\Phi}_e \rangle dt, \\
(6) \quad \frac{d^2 E(\Phi)}{du^2} &= -2 \sum_{x \in V} \langle D_W W(x), \sum_{e \in E_x} m_E(e) \dot{\Phi}_e(0) \rangle \\
&\quad + \sum_{e \in E} m_E(e) \int_0^1 \left(-\langle D_{W_e} W_e, \frac{D}{dt} \dot{\Phi}_e \rangle \right. \\
&\quad \quad \left. + \left\| \frac{D W_e}{dt} \right\|^2 - \langle W_e, R(W_e, \dot{\Phi}_e) \dot{\Phi}_e \rangle \right) dt,
\end{aligned}$$

where $E_x = \{e \in E \mid o(e) = x\}$ and R denotes the curvature tensor.

Proof. By routine computation, we have

$$(7) \quad \frac{dE(\Phi)}{du} = \sum_{e \in E} m_E(e) \left(\left\langle \frac{\partial \Phi_e}{\partial u}, \frac{\partial \Phi_e}{\partial t} \right\rangle \Big|_{t=0}^{t=1} - \int_0^1 \left\langle \frac{\partial \Phi_e}{\partial u}, \frac{D}{dt} \frac{\partial \Phi_e}{\partial t} \right\rangle dt \right).$$

Since

$$(8) \quad \frac{\partial \Phi_{\bar{e}}}{\partial u}(0, 1) = \frac{\partial \Phi_e}{\partial u}(0, 0) = W(o(e)), \quad \frac{\partial \Phi_{\bar{e}}}{\partial t}(0, 1) = -\frac{\partial \Phi_e}{\partial t}(0, 0) = -\dot{\Phi}_e(0),$$

$$\begin{aligned}
(9) \quad \sum_{e \in E} m_E(e) \left\langle \frac{\partial \Phi_e}{\partial u}, \frac{\partial \Phi_e}{\partial t} \right\rangle(0, 1) \\
= \sum_{e \in E} m_E(\bar{e}) \left\langle \frac{\partial \Phi_{\bar{e}}}{\partial u}, \frac{\partial \Phi_{\bar{e}}}{\partial t} \right\rangle(0, 1) = - \sum_{e \in E} m_E(e) \left\langle \frac{\partial \Phi_e}{\partial u}, \frac{\partial \Phi_e}{\partial t} \right\rangle(0, 0),
\end{aligned}$$

we find that

$$(10) \quad \frac{dE(\Phi)}{du}(0) = - \sum_{e \in E} m_E(e) \left(2 \langle W(o(e)), \dot{\Phi}_e(0) \rangle + \int_0^1 \langle W_e, \frac{D}{dt} \dot{\Phi}_e \rangle dt \right),$$

from which the first variation formula easily follows.

By a similar argument, we obtain the second variation formula

$$\begin{aligned}
(11) \quad \frac{d^2 E(\Phi)}{du^2}(0) &= \sum_{e \in E} m_E(e) \left(\left\langle D_{W_e} W_e, \dot{\Phi}_e \right\rangle \Big|_{t=0}^{t=1} + \int_0^1 \left(-\langle D_{W_e} W_e, \frac{D}{dt} \dot{\Phi}_e \rangle \right. \right. \\
&\quad \left. \left. + \left\| \frac{D W_e}{dt} \right\|^2 - \langle W_e, R(W_e, \dot{\Phi}_e) \dot{\Phi}_e \rangle \right) dt \right) \\
&= -2 \sum_{x \in V} \langle D_W W(x), \sum_{e \in E_x} m_E(e) \dot{\Phi}_e \rangle \\
&\quad + \sum_{e \in E} m_E(e) \int_0^1 \left(-\langle D_{W_e} W_e, \frac{D}{dt} \dot{\Phi}_e \rangle \right. \\
&\quad \quad \left. + \left\| \frac{D W_e}{dt} \right\|^2 - \langle W_e, R(W_e, \dot{\Phi}_e) \dot{\Phi}_e \rangle \right) dt.
\end{aligned}$$

□

Applying the first variation formula, we obtain

Theorem 2.2. *A piecewise smooth map Φ is a critical map if and only if Φ is a piecewise geodesic map, i.e. Φ_e is a geodesic for every edge e , and at each $x \in V$*

$$(12) \quad \sum_{e \in E_x} m_E(e) \dot{\Phi}_e(0) = 0.$$

A piecewise geodesic map of a general weighted graph X into Y satisfying (12) is called *harmonic*.

Remark. The energy of a piecewise geodesic map Φ is equal to

$$(13) \quad E(\Phi) = \frac{1}{2} \sum_{e \in E} m_E(e) \ell(e)^2,$$

where $\ell(e)$ is the length of the geodesic Φ_e .

In the special case when the target manifold Y is the Euclidean space \mathbb{R}^n , a piecewise geodesic map Φ of X into Y is uniquely determined by its restriction to the set of vertices, and the condition (12) is rewritten as

$$(14) \quad \sum_{e \in E_x} m_E(e) (\Phi(t(e)) - \Phi(o(e))) = 0,$$

since $\dot{\Phi}_e(0) = \Phi(t(e)) - \Phi(o(e))$.

Define the *discrete Laplacian* Δ acting on vector-valued functions on the set of vertices by

$$(15) \quad \Delta f(x) = m_V(x)^{-1} \sum_{e \in E_x} m_E(e) (f(t(e)) - f(o(e))).$$

With this terminology, (14) is rephrased as

$$(16) \quad \Delta \Phi = 0.$$

Namely, each component of the vector-valued function Φ is a harmonic function.

An easy remark is that, for a given affine map $A : \mathbb{R}^n \rightarrow \mathbb{R}^m$ and a function $\Phi : X \rightarrow \mathbb{R}^n$, we have $\Delta(A\Phi) = A\Delta\Phi$, and hence if Φ is harmonic, then so is $A\Phi$.

We may easily show that the *maximum principle* holds for the discrete Laplacian, namely that a real-valued harmonic function which attains its maximum (or minimum) is constant. In particular, real-valued harmonic functions on a finite weighted graph are constant. We now establish the following fundamental theorem.

Theorem 2.3. *Let X be a finite weighted graph, and let Y be a compact Riemannian manifold. Then each homotopy class of maps of X into Y contains at least one harmonic map.*

Proof. Let C be a homotopy class of maps of X into Y . For each piecewise smooth map $\Phi \in C$, one can find a piecewise geodesic map $\Phi_1 \in C$ with $E(\Phi_1) \leq E(\Phi)$. Indeed, it is enough to replace each Φ_e by the shortest geodesic homotopic to Φ_e relative to the end points. We denote by C^* the set of piecewise geodesic maps in C , and on it we introduce the C^1 -topology so that the functional E is continuous on C^* . It is straightforward to see that, for every $a > 0$, the sublevel set $\{\Phi \in C^* \mid E(\Phi) \leq a\}$ is compact. Therefore one can find a $\Phi_0 \in C^*$ such that $E(\Phi_0) \leq E(\Phi)$ for every $\Phi \in C^*$. Since Φ_0 is a critical map, it gives a desired harmonic map. \square

The following theorem asserts the uniqueness of harmonic maps in a fixed homotopy class of maps into a flat torus.

Theorem 2.4. *Let g_1 and g_2 be flat metrics on a torus \mathcal{T} , and let X be a finite weighted graph. If two harmonic maps $\Phi_1 : X \rightarrow (\mathcal{T}, g_1)$ and $\Phi_2 : X \rightarrow (\mathcal{T}, g_2)$ are homotopic, then there exists an element $a \in \mathcal{T}$ such that $\Phi_1 - \Phi_2 \equiv a$.*

Proof. Write $\mathcal{T} = \mathbb{R}^n/\Gamma$ with a lattice subgroup Γ of \mathbb{R}^n , and let $\tilde{\Phi}_i : \tilde{X} \rightarrow \mathbb{R}^n$ be a lift of the harmonic map Φ_i to the universal covering graph $\tilde{X} = (\tilde{V}, \tilde{E})$ of X for $i = 1, 2$. Denote by $\rho : \pi_1(X) \rightarrow \Gamma$ the homomorphism induced from the map Φ_i . We find that

$$(17) \quad \tilde{\Phi}_i(\sigma\tilde{x}) = \tilde{\Phi}_i(\tilde{x}) + \rho(\sigma)$$

for $\tilde{x} \in \tilde{X}$ and $\sigma \in \pi_1(X)$, and hence $\tilde{\Phi}_1 - \tilde{\Phi}_2$ is a $\pi_1(X)$ -invariant function on \tilde{X} . The function $\tilde{\Phi}_1 - \tilde{\Phi}_2$ is harmonic because the condition for a map of \tilde{X} into \mathbb{R}^n to be harmonic does not depend on the choice of flat metrics on \mathbb{R}^n . Therefore $\tilde{\Phi}_1 - \tilde{\Phi}_2$ is a lift of a harmonic function on X , and hence we conclude, in view of the maximum principle, that there exists $\tilde{a} \in \mathbb{R}^n$ such that $\tilde{\Phi}_1 - \tilde{\Phi}_2 \equiv \tilde{a}$. This completes the proof. \square

Theorem 2.5. *Let Y be a compact Riemannian manifold with non-positive sectional curvature, and let C be a homotopy class of maps from a finite weighted graph X into Y . Then a map $\Phi \in C$ is harmonic if and only if Φ minimizes the energy functional restricted to C . Furthermore, if Y has strictly negative sectional curvature, and if a map in C induces a homomorphism of $\pi_1(X)$ into $\pi_1(Y)$ whose image is not cyclic, then C contains a unique harmonic map.*

Proof. Let Φ_0 and Φ_1 be harmonic maps in C . One may choose lifts $\tilde{\Phi}_0, \tilde{\Phi}_1 : \tilde{X} \rightarrow \tilde{Y}$ of Φ_0, Φ_1 to the universal covering spaces, respectively, satisfying

$$(18) \quad \tilde{\Phi}_i(\sigma\tilde{x}) = \rho(\sigma)\tilde{\Phi}_i(\tilde{x}) \quad (\sigma \in \pi_1(X); \tilde{x} \in \tilde{X}; i = 0, 1)$$

with the same induced homomorphism $\rho : \pi_1(X) \rightarrow \pi_1(Y)$. Joining $\tilde{\Phi}_0(\tilde{x})$ and $\tilde{\Phi}_1(\tilde{x})$ by a unique geodesic in \tilde{Y} , one may define a piecewise smooth map $\tilde{\Phi}_u : \tilde{X} \rightarrow \tilde{Y}$ for $0 \leq u \leq 1$. It is easy to check that $\tilde{\Phi}_u(\sigma\tilde{x}) = \rho(\sigma)\tilde{\Phi}_u(\tilde{x})$, so that one has a piecewise smooth map $\Phi_u : X \rightarrow Y$ in C whose lift is $\tilde{\Phi}_u$. Applying the second variation formula, we observe that $d^2E(\Phi_u)/du^2 \geq 0$ for $D_{W_e}W_e = 0$. Since

$$(19) \quad \left. \frac{dE(\Phi_u)}{du} \right|_{u=0} = \left. \frac{dE(\Phi_u)}{du} \right|_{u=1} = 0,$$

we find that $dE(\Phi_u)/du \equiv 0$, and hence $E(\Phi_u) \equiv \text{constant}$. This implies the first assertion.

For the second assertion, we first observe from the second variation formula and nonpositivity of the curvature that $DW_e/dt \equiv 0$ and $\langle R(W_e, \dot{\Phi}_e(0))\dot{\Phi}_e(0), W_e \rangle \equiv 0$ since $d^2E(\Phi_u)/du^2 \equiv 0$. From the assumption that the curvature is strictly negative, it follows that $W(x) = c\dot{\Phi}_e(0)$ with some constant c . Since the image of ρ is not cyclic, there exists a vertex x of X such that the dimension of the subspace spanned by $\{\dot{\Phi}_e(0) \mid e \in E_x\}$ is greater than one. Indeed, if the dimension is one or zero for every vertex, then the image of Φ lies in a circle in Y so that the image of ρ is cyclic; this is a contradiction. Thus $W_e \equiv 0$ for $e \in E_x$, and hence for all $e \in E$ because $DW_e/dt \equiv 0$. This implies that $\Phi_1 = \Phi_2$, as desired. \square

Given an n -dimensional compact smooth manifold N , we consider a family \mathcal{G} of Riemannian metrics on N with a fixed volume. Take a homotopy class C of maps of a finite weighted graph X into N , and consider the function $E = E(\Phi, g)$ on $C \times \mathcal{G}$. Closely related to the subject in this paper is the following general problem. *Does the function E attain its minimum at some pair (Φ_0, g_0) ?* Actually the first part of Theorem 2 says that this is the case when N is a torus, \mathcal{G} is the family of flat metrics on N , and maps in C induce a surjective homomorphism of $\pi_1(X)$ onto $\pi_1(N)$. It is rather easy, in this special case, to show the existence of such a pair. The core of our problem is to detect (Φ_0, g_0) in an explicit way.

It is interesting to investigate the case of a surface N with the family \mathcal{G} of constant negatively curved metrics, which is regarded as a non-Euclidean analogue of our problem in dimension two.

Remark. Recently much attention has been paid to harmonic maps between singular metric spaces including graphs (see [4],[5],[6],[10],[12] for instance). Actually the existence of energy minimizing harmonic maps of a finite weighted graph into a *fixed* flat torus is a very special case of the results in more general situations [6].

We should also remark that in [3], Ejiri studied the index of compact minimal surfaces in tori by looking at the variation of flat structures of tori.

3. REDUCTION TO A GEOMETRIC PROBLEM

We shall explain briefly how Theorem 1 is reduced to the problem in terms of flat tori and weighted graphs as stated in Theorem 2.

With a system of springs in \mathbb{R}^n , one may always associate a graph in such a way that the springs correspond to unoriented edges and the points of masses correspond to vertices, where the incidence of edges and vertices is defined in a natural manner. The two atoms connected by a spring are supposed to interact each other by the dynamical law of a harmonic oscillator. Regarding the masses and the force constants as weights of vertices and edges respectively, we have a weighted graph. Furthermore, joining two adjacent vertices by the line segment, we have a piecewise geodesic map Φ from the graph into the Euclidean space, where $\Phi(x)$ designates the position of a mass x . The force acting on the mass x generated by the spring e with $o(e) = x$ is given by $m_E(e)(\Phi(t(e)) - \Phi(o(e)))$, where $m_E(e)$ is the force constant of the spring e . By the principle of superposition, we conclude that the total force acting on the mass x is given by

$$(20) \quad \sum_{e \in E_x} m_E(e)(\Phi(t(e)) - \Phi(o(e))).$$

Therefore, in view of (14), the internal forces in the system of springs is in equilibrium if and only if Φ is harmonic. For a finite system of springs, $E(\Phi)$ coincides with the potential energy of the system. It is worth mentioning that the vibration of the system is described by Newton's dynamical equation

$$(21) \quad \frac{d^2\Phi}{dt^2} = \Delta\Phi,$$

which is regarded as a discrete analogue of the wave equation.

Consider the system of springs corresponding to a crystal in \mathbb{R}^n , which need not have the equilibrium configuration. The additive group Γ of translations acting on the system is a lattice group, known as the Bravais lattice, namely a group

consisting of vectors \mathbf{x} represented as integral linear combinations of n linearly independent vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n$:

$$\Gamma = \left\{ \mathbf{x} = \sum_{i=1}^n k_i \mathbf{v}_i \mid k_i \text{ integers} \right\}.$$

As a primitive unit cell of the crystal, we may take a fundamental parallelootope P in the space for the action of Γ , that is,

$$P = \left\{ \mathbf{x} = \sum_{i=1}^n a_i \mathbf{v}_i \mid 0 \leq a_i < 1 \right\}.$$

We identify P with the torus $T_\Gamma = \mathbb{R}^n / \Gamma$. The torus T_Γ has the flat metric induced from the one on the Euclidean space \mathbb{R}^n . The volume of the primitive unit cell is nothing but the volume $\text{vol}(T_\Gamma)$ of the flat torus T_Γ as a Riemannian manifold. It should be noted here that

$$(22) \quad \text{vol}(T_\Gamma) = \text{vol}(P) = (\det(\langle \mathbf{v}_i, \mathbf{v}_j \rangle))^{1/2}.$$

On the other hand, we identify two masses in the system if one of them is obtained by translation in Γ from the other. We also identify two springs in the same way. We thus have a finite system of springs, which is realized in the flat torus T_Γ .

Applying the general recipe above to the system associated with a crystal, we obtain two weighted graphs, one of which, denoted by X , corresponds to the crystal itself and the other, denoted by X_0 , corresponds to the finite system realized in the flat torus. The piecewise geodesic map Φ gives a *configuration* of the crystal. The piecewise geodesic map Φ_0 of X_0 into T_Γ is the one obtained by projecting down the map Φ to X_0 . From the construction, it follows that Φ_0 is harmonic if and only if Φ is harmonic. Therefore the internal forces in the crystal are *in equilibrium* if and only if the map Φ_0 is harmonic. We define the potential energy per primitive unit cell as the energy of Φ_0 .

The graph X is called the *crystal lattice*. The lattice group Γ acts on X as a graph automorphism. In the context of graph theory, X_0 is the *quotient graph* of X by the action of Γ . From now on, we consider Γ as an abstract group acting on X . When a configuration of the crystal varies, T_Γ , the primitive unit cell, changes, although its topological type does not. In other words, according as the piecewise geodesic map Φ_0 varies, the flat metric g on the torus changes. Therefore we paraphrase our problem with this terminology in the following way. Fix a topological torus \mathcal{T} and a homotopy class C of maps from X_0 to \mathcal{T} , and let $v_0 > 0$. An *equilibrium configuration* of the crystal is a lift of a pair (Φ_0, g_0) which minimizes the energy $E = E(\Phi, g)$ under the condition that $\Phi_0 \in C$ and $\text{vol}(\mathcal{T}, g) = v_0$, where, from its nature, the homotopy class C is supposed to satisfy the condition that a map in C induces the surjective homomorphism of $\pi_1(X_0)$ onto $\pi_1(\mathcal{T})$. We are thus led to the setup described in Theorem 2. It should be noted that the masses of atoms do not play any role as far as the static nature of crystals is concerned.

We shall illustrate the above discussion by taking a look at the diamond crystal. For simplicity, the weights of vertices and edges are taken to be one. Let $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ be the standard basis of \mathbb{R}^3 . We consider the lattice group Γ generated by the basis $\mathbf{v}_1 = \mathbf{e}_2 + \mathbf{e}_3 = (0, 1, 1)$, $\mathbf{v}_2 = \mathbf{e}_3 + \mathbf{e}_1 = (1, 0, 1)$, $\mathbf{v}_3 = \mathbf{e}_1 + \mathbf{e}_2 = (1, 1, 0)$. Γ is what we call the *face centered cubic lattice group*. It is easy to check that $\text{vol}(T_\Gamma) = 2$.

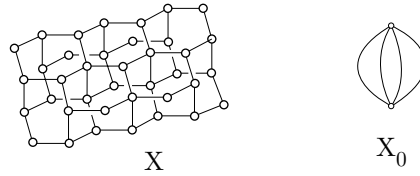


FIGURE 1. The diamond lattice and its quotient graph

The sites of carbon atoms are divided into two kinds:

$$A = \Gamma = \{(m_2 + m_3, m_3 + m_1, m_1 + m_2) \mid m_i \in \mathbb{Z}\},$$

$$B = (1/2, 1/2, 1/2) + \Gamma$$

$$= \{(n_2 + n_3 + 1/2, n_3 + n_1 + 1/2, n_1 + n_2 + 1/2) \mid n_i \in \mathbb{Z}\}.$$

Two atoms at sites $(m_2 + m_3, m_3 + m_1, m_1 + m_2)$, $(n_2 + n_3 + 1/2, n_3 + n_1 + 1/2, n_1 + n_2 + 1/2)$ are to be bonded by an edge if and only if one of the followings holds:

$$\begin{aligned} m_1 &= n_1, & m_2 &= n_2, & m_3 &= n_3, \\ m_1 &= n_1 + 1, & m_2 &= n_2, & m_3 &= n_3, \\ m_1 &= n_1, & m_2 &= n_2 + 1, & m_3 &= n_3, \\ m_1 &= n_1, & m_2 &= n_2, & m_3 &= n_3 + 1, \end{aligned}$$

In this way, we have a crystal lattice X for a diamond, which we call the *diamond lattice*. It should be noted that the origin \mathbf{o} is in A , and the vertices in the nearest neighbor of \mathbf{o} are

$$(23) \quad \begin{aligned} \mathbf{a}_1 &= (1/2, 1/2, 1/2), \\ \mathbf{a}_2 &= (1/2, -1/2, -1/2), \\ \mathbf{a}_3 &= (-1/2, 1/2, -1/2), \\ \mathbf{a}_4 &= (-1/2, -1/2, 1/2). \end{aligned}$$

We observe that $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4$ form the regular tetrahedron whose center of mass is \mathbf{o} . It is also easily checked that the quotient graph X_0 is the graph with two vertices joined by 3 multiple edges. The potential energy per primitive unit cell is equal to 3. We shall show in §5 that this configuration is the equilibrium configuration.

4. THE STANDARD REALIZATION OF GENERALIZED CRYSTAL LATTICES

We shall set up the class of graphs which generalizes the notion of crystal lattices.

A locally finite connected weighted graph $X = (V, E)$ with weight functions m_V and m_E is said to be a *generalized crystal lattice* or Γ -*crystal lattice* if the following conditions are satisfied.

1. There exists a free abelian automorphism group Γ of X which acts freely on the set V and the set of unoriented edges.
2. The weight functions are Γ -invariant.
3. The quotient graph $\Gamma \backslash X = X_0$ is finite.

In other words, X is an abelian covering graph of a finite weighted graph X_0 with the covering transformation group Γ , and the weight functions on X are the lifts of those on X_0 .

The weighted graph associated with a crystal which we considered in §3 is a Γ -crystal lattice with the Bravais lattice Γ .

Let X be a Γ -crystal lattice with the quotient graph $X_0 = \Gamma \backslash X$. Let $\varphi : X \rightarrow X_0$ be the covering map and let $\varphi^{ab} : X_0^{ab} \rightarrow X_0$ be the maximal abelian covering map with the covering transformation group $H_1(X_0, \mathbb{Z})$, the 1-homology group with coefficients in \mathbb{Z} . Then there exists a covering map $\varphi_1 : X_0^{ab} \rightarrow X$ such that $\varphi \circ \varphi_1 = \varphi^{ab}$.

We shall introduce several inner product spaces over \mathbb{R} associated with the finite weighted graph X_0 . We adopt the following convention throughout this section. Given an inner product space \mathcal{V} , the dual vector space and quotient vector spaces of \mathcal{V} are considered as inner product spaces with the canonical inner products obtained from that of \mathcal{V} .

We denote by $C^i(X_0, \mathbb{R})$ the i -th cochain group ($i = 0, 1$) of the finite graph $X_0 = (V_0, E_0)$ with the following inner product:

$$(24) \quad \begin{aligned} \langle f_1, f_2 \rangle &= \sum_{x \in V_0} m_{V_0}(x) f_1(x) f_2(x) & (f_1, f_2 \in C^0(X_0, \mathbb{R})), \\ \langle \omega_1, \omega_2 \rangle &= \frac{1}{2} \sum_{e \in E_0} m_{E_0}(e) \omega_1(e) \omega_2(e) & (\omega_1, \omega_2 \in C^1(X_0, \mathbb{R})). \end{aligned}$$

The adjoint operator $\delta : C^1(X_0, \mathbb{R}) \rightarrow C^0(X_0, \mathbb{R})$ of the coboundary operator $d : C^0(X_0, \mathbb{R}) \rightarrow C^1(X_0, \mathbb{R})$ is given by

$$(25) \quad (\delta\omega)(x) = -m_{V_0}(x)^{-1} \sum_{e \in (E_0)_x} \omega(e) m_{E_0}(e).$$

The operators d and δ extend to vector-valued cochains in a natural manner.

It should be noted that $\Delta = -\delta d$. Since $(\text{Image } d)^\perp = \text{Ker } \delta$, we may identify the 1-cohomology group $H^1(X_0, \mathbb{R})$, which is the quotient inner product space $C^1(X_0, \mathbb{R}) / \text{Image } d$, with the subspace $\text{Ker } \delta$ of $C^1(X_0, \mathbb{R})$, the space of ‘‘harmonic 1-forms’’. Next we consider the i -th chain group $C_i(X_0, \mathbb{R})$, which is considered to be the dual inner product space of $C^i(X_0, \mathbb{R})$. More explicitly, the inner product \cdot on $C_1(X_0, \mathbb{R})$ is given by

$$(26) \quad e \cdot e' = \begin{cases} m_{E_0}(e)^{-1}, & e = e', \\ -m_{E_0}(e)^{-1}, & e = \bar{e}', \\ 0, & \text{otherwise.} \end{cases}$$

Let X be a Γ -crystal lattice with the quotient graph X_0 . We extend the homomorphism $\rho : H_1(X_0, \mathbb{Z}) \rightarrow \Gamma$ associated with the covering map $\varphi : X \rightarrow X_0$ to the linear map $\rho_{\mathbb{R}} : H_1(X_0, \mathbb{R}) = H_1(X_0, \mathbb{Z}) \otimes \mathbb{R} \rightarrow \Gamma \otimes \mathbb{R}$. Note that $\rho_{\mathbb{R}}(H_1(X_0, \mathbb{Z})) = \Gamma$. We regard $\Gamma \otimes \mathbb{R}$ as a quotient inner product space of $H_1(X_0, \mathbb{R})$ and denote the inner product by $\langle \cdot, \cdot \rangle_{alb}$. The flat metric on the torus $\Gamma \otimes \mathbb{R} / \Gamma$ induced from $\langle \cdot, \cdot \rangle_{alb}$ is called the *Albanese metric* and is denoted by g_{alb} . We write Alb^Γ for $(\Gamma \otimes \mathbb{R} / \Gamma, g_{alb})$, and call it the Γ -*Albanese torus*. In the case of the maximal abelian covering graph,

$$(27) \quad \text{Alb}^\Gamma = \text{Alb}(X_0) = H_1(X_0, \mathbb{R}) / H_1(X_0, \mathbb{Z}).$$

The transpose $\rho_{\mathbb{R}}^*$ of $\rho_{\mathbb{R}}$ is an injective map of $\text{Hom}(\Gamma, \mathbb{R}) = (\Gamma \otimes \mathbb{R})^*$ into $H^1(X_0, \mathbb{R})$. From now on, we consider $\text{Hom}(\Gamma, \mathbb{R})$ as a subspace of $H^1(X_0, \mathbb{R})$ via $\rho_{\mathbb{R}}^*$.

We shall define a harmonic map $\Phi^\Gamma : X_0 \rightarrow Alb^\Gamma$. For this, we first define $\tilde{\Phi}^\Gamma : V \rightarrow \Gamma \otimes \mathbb{R}$ by

$$(28) \quad \tilde{\Phi}^\Gamma(x)(\omega) = \int_{x_0}^x \tilde{\omega},$$

where $\tilde{\omega}$ is the lift of a harmonic 1-form $\omega \in \text{Hom}(\Gamma, \mathbb{R}) \subset H^1(X_0, \mathbb{R})$ and the integral in the right hand side is defined, for a path $c = (e_1, \dots, e_l)$ with $o(c) = x_0, t(c) = x$, by

$$(29) \quad \int_{x_0}^x \tilde{\omega} = \tilde{\omega}(e_1) + \dots + \tilde{\omega}(e_l).$$

It should be noted that $\tilde{\Phi}^\Gamma(x)(\omega)$ does not depend on the choice of a path c . Next we put, for each $e \in E$,

$$(30) \quad \tilde{\Phi}_e^\Gamma(t) = \tilde{\Phi}^\Gamma(e, t) = (1 - t)\tilde{\Phi}^\Gamma(o(e)) + t\tilde{\Phi}^\Gamma(t(e)).$$

In this way, we have a piecewise geodesic map $\tilde{\Phi}^\Gamma : X \rightarrow \Gamma \otimes \mathbb{R}$. Note that, for $\sigma \in \Gamma$,

$$(31) \quad \tilde{\Phi}^\Gamma(\sigma x) = \tilde{\Phi}^\Gamma(x) + \sigma,$$

since $\int_{x_0}^{\sigma x_0} \tilde{\omega} = \omega(\sigma)$, and for every $\omega \in \text{Hom}(\Gamma, \mathbb{R})$,

$$(32) \quad \sum_{e \in E_x} m_E(e)(\tilde{\Phi}^\Gamma(t(e)) - \tilde{\Phi}^\Gamma(o(e)))(\tilde{\omega}) = \sum_{e \in E_x} m_E(e)\tilde{\omega}(e) = 0.$$

We thus obtain a harmonic map $\Phi^\Gamma : X_0 \rightarrow Alb^\Gamma$.

The map Φ^Γ is an analogue of the Albanese maps, which were originally defined in algebraic geometry and Riemannian geometry (see [9]). The image $\tilde{\Phi}^\Gamma$ is called the *standard realization* of the generalized crystal lattice X .

Let X be a Γ -crystal lattice with X_0 as its quotient graph, and let $\tau : \Gamma \rightarrow \Gamma_1$ be a surjective homomorphism onto a free abelian group Γ_1 . The quotient graph $\text{Ker } \tau \backslash X$ is a Γ_1 -crystal graph with X_0 as its quotient graph. The inner product space $\Gamma_1 \otimes \mathbb{R}$ is a quotient inner product space of $\Gamma \otimes \mathbb{R}$ via the linear map $\tau_{\mathbb{R}} : \Gamma \otimes \mathbb{R} \rightarrow \Gamma_1 \otimes \mathbb{R}$ induced from τ . We thus obtain a Riemannian submersion $\tau_* : Alb^\Gamma \rightarrow Alb^{\Gamma_1}$ in a natural manner. We may easily check that $\tau_{\mathbb{R}} \circ \tilde{\Phi}^\Gamma = \tilde{\Phi}^{\Gamma_1} \circ \varphi_1$ and $\tau_* \circ \Phi^\Gamma = \Phi^{\Gamma_1}$, where $\varphi_1 : X \rightarrow X_1$ denotes the canonical projection. In particular, applying this discussion to the homomorphism $\rho : H_1(X_0, \mathbb{Z}) \rightarrow \Gamma$ associated with the covering map $\varphi : X \rightarrow X_0$, we find that the standard realization of X in $\Gamma \otimes \mathbb{R}$ coincides with the image of the standard realization for the maximal abelian covering X_0^{ab} in $H_1(X_0, \mathbb{R})$ by the orthogonal projection $\rho_{\mathbb{R}} : H_1(X_0, \mathbb{R}) \rightarrow \Gamma \otimes \mathbb{R}$.

Next, we let Γ_1 be a subgroup of Γ with finite index ℓ . A Γ -crystal lattice X is also considered as a Γ_1 -crystal lattice with the finite quotient graph $X_1 = \Gamma_1 \backslash X$. The covering map $\varphi : X \rightarrow X_0$ is factored as

$$(33) \quad X \xrightarrow{\varphi_1} X_1 \xrightarrow{\varphi_0} X_0,$$

where φ_0 is an ℓ -fold covering map. Let $\iota : \Gamma_1 \rightarrow \Gamma$ be the inclusion map. We observe that the linear map $\iota_{\mathbb{R}} : \Gamma_1 \otimes \mathbb{R} \rightarrow \Gamma \otimes \mathbb{R}$ satisfies

$$(34) \quad \langle \iota_{\mathbb{R}}(\mathbf{u}), \iota_{\mathbb{R}}(\mathbf{v}) \rangle_{alb} = \ell \langle \mathbf{u}, \mathbf{v} \rangle_{alb},$$

and induces a homothetic ℓ -fold covering map $\iota_* : Alb_1^\Gamma \rightarrow Alb^\Gamma$. From the construction of Albanese maps, we find that $\iota_{\mathbb{R}} \circ \tilde{\Phi}^{\Gamma_1} = \tilde{\Phi}^\Gamma$ and $\iota_* \circ \Phi^{\Gamma_1} = \Phi^\Gamma \circ \varphi_0$.

This implies that the standard realization of the crystal lattice X up to homothety depends only on the commensurable class of groups Γ . It is easily checked that $\text{vol}(\text{Alb}^\Gamma) = \ell^{k/2-1} \text{vol}(\text{Alb}_1^\Gamma)$, where $k = \text{rank } \Gamma = \text{rank } \Gamma_1$.

We shall now see that the Albanese map $\Phi^\Gamma : X_0 \rightarrow \text{Alb}^\Gamma$ is characterized as a map with minimal energy among piecewise smooth maps, which is homotopic to Φ^Γ , of X_0 into the torus $\Gamma \otimes \mathbb{R}/\Gamma$ with a flat metric whose volume is the same as $\text{vol}(\text{Alb}^\Gamma)$.

Theorem 4.1. *Let g be a flat metric on the torus $\mathcal{T} = \Gamma \otimes \mathbb{R}/\Gamma$ with the same volume as g_{alb} , and let Φ be a piecewise smooth map from X_0 to (\mathcal{T}, g) . If Φ is homotopic to Φ^Γ , then*

$$E(\Phi^\Gamma, g_{\text{alb}}) \leq E(\Phi, g).$$

The equality holds if and only if $(\mathcal{T}, g) = (\mathcal{T}, g_{\text{alb}}) = \text{Alb}^\Gamma$ and Φ coincides with Φ^Γ up to a translation.

We preface the proof with two lemmas.

A *path* in a graph is a sequence $c = (e_1, \dots, e_l)$ with $t(e_i) = o(e_{i+1}), i = 1, \dots, l-1$. We put $o(c) = o(e_1), t(c) = t(e_l)$. When $o(c) = t(c)$, the path c is said to be *closed*. A closed path without self-intersections is called a *circuit*.

Given a circuit $c = (e_1, \dots, e_l)$ in X_0 , we define a cochain ω_c by

$$(35) \quad \omega_c(e) = \begin{cases} m_{E_0}(e_i)^{-1}, & e = e_i, \\ -m_{E_0}(e_i)^{-1}, & \bar{e} = e_i, \\ 0, & \text{otherwise.} \end{cases}$$

We observe that ω_c is a harmonic 1-form and

$$(36) \quad \langle \omega_{c_1}, \omega_{c_2} \rangle = \omega_{c_1}(c_2) = c_1 \cdot c_2.$$

An *orientation* of X_0 is given by a subset E_0^o of E_0 such that $E_0 = E_0^o \amalg \overline{E_0^o}$, where $\overline{E_0^o} = \{\bar{e} \mid e \in E_0^o\}$. Let N be the number of vertices and M the number of unoriented edges of X_0 .

Lemma 4.2. *There exists a \mathbb{Z} -basis c_1, \dots, c_n of the 1-homology group $H_1(X_0, \mathbb{Z})$ ($n = \text{rank } H_1(X_0, \mathbb{Z})$) consisting of circuits.*

Proof. Take a maximal (spanning) tree $T = (V_T, E_T)$ of X_0 , a maximal element among subtrees ordered by inclusion. The tree T contains all vertices of X_0 , and the number of the unoriented edges not contained in T is equal to n . Give an orientation $E_0^o = \{e_1, \dots, e_M\}$ to the graph X_0 such that

$$(37) \quad \begin{aligned} e_1, \dots, e_n &\notin E_T, \\ e_{n+1}, \dots, e_M &\in E_T. \end{aligned}$$

For i with $1 \leq i \leq n$, take the minimal path c'_i in T such that $o(c'_i) = t(e_i), t(c'_i) = o(e_i)$, and put $c_i = e_i c'_i$. We easily find that the circuits c_1, \dots, c_n form a basis of $H_1(X_0, \mathbb{R})$. \square

Let c_1, \dots, c_n be a \mathbb{Z} -basis of the 1-homology group $H_1(X_0, \mathbb{Z})$ consisting of circuits, and let $u_1, \dots, u_n \in H^1(X_0, \mathbb{R})$ be the dual basis, i.e. $u_i(c_j) = \delta_{ij}$. Put

$\omega_i = \omega_{c_i}$. Then $\omega_1, \dots, \omega_n$ form an \mathbb{R} -basis of $H^1(X_0, \mathbb{R})$. Therefore one can find an $n \times n$ matrix $U = (u_{ij})$ such that

$$(38) \quad u_i = \sum_{j=1}^n u_{ij} \omega_j.$$

Choose an orientation $E_0^o = \{e_1, \dots, e_M\}$ of X_0 and put $W = \text{diag}(\mu_1, \dots, \mu_M)$ with $\mu_i = m_E(e_i)^{-1}$. Writing $c_i = \sum_{l=1}^M f_{il} e_l$, we define an $n \times M$ matrix $F = (f_{il})$. It is easy to check

Lemma 4.3. *Put $\Lambda = (c_i \cdot c_j)$. Then*

$$(39) \quad \Lambda = U^{-1},$$

$$(40) \quad \Lambda = FW F^t.$$

Proof. The first equality follows from

$$(41) \quad \delta_{ij} = u_i(c_j) = \sum_{h=1}^n u_{ih} \omega_h(c_j) = \sum_{h=1}^n u_{ih} \Lambda_{hj}.$$

The second one is checked as

$$(42) \quad \begin{aligned} c_i \cdot c_j &= \left(\sum_{l=1}^M f_{il} e_l \right) \cdot \left(\sum_{m=1}^M f_{jm} e_m \right) \\ &= \sum_{l,m=1}^M f_{il} f_{jm} e_l \cdot e_m = \sum_{l=1}^M f_{il} \mu_l f_{jl}. \end{aligned}$$

□

Now we are ready to prove Theorem 4.1.

Proof. We may assume Φ is harmonic because a harmonic map into a torus with a fixed flat metric is energy minimizing (Theorem 2.5). Owing to Theorem 2.4, Φ is equal to Φ^Γ up to a translation as a map to $\mathcal{T} = \Gamma \otimes \mathbb{R} / \Gamma$, and we only have to find a flat metric g on \mathcal{T} with a fixed volume which minimizes the energy $E(\Phi^\Gamma, g)$. We shall show that such a metric is homothetic to the Albanese metric. Without loss of generality, we may assume that $\text{vol}(\mathcal{T}, g) = \text{vol}(\mathcal{T}, g_{\text{alb}})$.

Take a \mathbb{Z} -basis $\sigma_1, \dots, \sigma_k$ of Γ , and let $v_1, \dots, v_k \in \text{Hom}(\Gamma, \mathbb{R})$ be the dual basis of $\sigma_1, \dots, \sigma_k$, where $k = \text{rank } \Gamma$. Write

$$(43) \quad c'_i = \rho_{\mathbb{R}}(c_i) = \sum_{j=1}^k r_{ji} \sigma_j \quad (r_{ji} \in \mathbb{Z}; i = 1, \dots, n).$$

Then we have $v_j = \rho_{\mathbb{R}}^*(v_j) = \sum_{i=1}^n r_{ji} u_i$. Put $S = (\langle v_i, v_j \rangle) = R U R^t$. Note that $S^{-1} = \langle \sigma_i, \sigma_j \rangle_{\text{alb}}$.

Regard $\tilde{\Phi} (= \tilde{\Phi}^\Gamma)$ as a 0-cochain of X with values in the vector space $\Gamma \otimes \mathbb{R}$. It is obvious that $d\tilde{\Phi} \in C^1(X, \Gamma \otimes \mathbb{R})$ satisfies $d\tilde{\Phi}(\sigma e) = d\tilde{\Phi}(e)$ for $e \in E$ and $\sigma \in \Gamma$. Therefore $d\tilde{\Phi}$ is identified with a 1-cochain of X_0 with values in $\Gamma \otimes \mathbb{R}$.

Put

$$(44) \quad \mathbf{v}_i = d\tilde{\Phi}(e_i) \quad \text{for } i = 1, \dots, M.$$

Now, for $\omega \in \text{Hom}(\Gamma, \mathbb{R}) \subset H^1(X_0, \mathbb{R})$, we have

$$(45) \quad \begin{aligned} \omega(e_i) &= \sum_j \langle \omega, u_j \rangle u_j(e_i) = \sum_j \omega(c_j) u_j(e_i) = \sum_j (\rho_{\mathbb{R}}^* \omega)(c_j) u_j(e_i) \\ &= \sum_j \omega(\rho_{\mathbb{R}}(c_j)) u_j(e_i) = \sum_j \omega(c'_j) u_j(e_i), \end{aligned}$$

and $\mathbf{v}_i(\omega) = \omega(e_i)$. Therefore we have

$$(46) \quad \begin{aligned} \mathbf{v}_i &= \sum_{j=1}^n u_j(e_i) c'_j = \sum_{j=1}^n \sum_{m=1}^n u_{jm} \omega_m(e_i) c'_j \\ &= \sum_{j=1}^n \sum_{m=1}^n u_{jm} f_{mi} \mu_i c'_j = \sum_{j=1}^n \sum_{m=1}^n \sum_{l=1}^k u_{jm} f_{mi} \mu_i r_{lj} \sigma_l \\ &= \sum_{l=1}^k (WF^t U R^t)_{il} \sigma_l. \end{aligned}$$

We put $A = (\langle \sigma_i, \sigma_j \rangle_g)$. Since

$$(47) \quad \text{vol}(\Gamma \otimes \mathbb{R}/\Gamma, g_{alb}) = (\det S)^{-1/2},$$

$$(48) \quad \text{vol}(\Gamma \otimes \mathbb{R}/\Gamma, g) = (\det A)^{1/2},$$

we have $\det(SA) = 1$.

The energy $E(\Phi^\Gamma, g)$ is computed in the following way:

$$(49) \quad \begin{aligned} E(\Phi^\Gamma, g) &= \sum_{i=1}^M m_E(e_i) \|\mathbf{v}_i\|_g^2 = \sum_{i=1}^M \sum_{j,h=1}^k \mu_i^{-1} (WF^t U R^t)_{ij} (WF^t U R^t)_{ih} A_{jh} \\ &= \text{tr}(F^t U R^t A (WF^t U R^t)^t) = \text{tr}(R U F W F^t U R^t A) \\ &= \text{tr}(R U \Lambda U R^t A) = \text{tr}(R U R^t A) = \text{tr}(SA). \end{aligned}$$

Let \sqrt{S} be the positive square root of the positive definite symmetric matrix S . Then we have

$$(50) \quad \text{tr}(SA) = \text{tr}(\sqrt{S} A \sqrt{S}) \geq k \det(\sqrt{S} A \sqrt{S})^{1/k} = k \det(SA)^{1/k} = k.$$

The equality holds if and only if $SA = I$, or equivalently

$$(51) \quad \langle \sigma_i, \sigma_j \rangle_g = \langle \sigma_i, \sigma_j \rangle_{alb},$$

i.e. $g = g_{alb}$. □

Since $E(\Phi^\Gamma, cg) = cE(\Phi^\Gamma, g)$ and $\text{vol}(cg) = c^{k/2} \text{vol}(g)$ for $c > 0$, the above proof leads us to the following

Theorem 4.4. *Let X be a k -dimensional crystal lattice with the Bravais lattice group Γ , and let \mathcal{E}_0 be the potential energy per primitive unit cell with volume v_0 . Then*

$$(52) \quad \mathcal{E}_0 v_0^{-2/k} \geq k \text{vol}(\text{Alb}^\Gamma)^{-2/k}.$$

The equality holds if and only if the configuration of X is in equilibrium.

So far we have explained how the equilibrium configurations of crystal lattices are described in terms of the Albanese maps into the Albanese tori. We are now in position to prove Theorem 2, which is actually a disguised form of Theorem 4.1.

Let C be a homotopy class of maps from a finite weighted graph X_0 into a torus (\mathcal{T}, g) which induces a surjective homomorphism $\eta : \pi_1(X_0) \rightarrow \pi_1(\mathcal{T})$. Put $\Gamma = \pi(X_0)/\text{Ker } \eta$ and $X = \text{Ker } \eta \backslash \tilde{X}_0$, where \tilde{X}_0 is the universal covering graph of X_0 . Then X is a Γ -crystal lattice with X_0 as its quotient graph.

Lemma 4.5. *There exists an affine isomorphism $\alpha : \Gamma \otimes \mathbb{R}/\Gamma \rightarrow \mathcal{T}$ such that $\alpha \circ \Phi^\Gamma \in C$.*

Proof. Identify \mathcal{T} with $H_1(\mathcal{T}, \mathbb{R})/H_1(\mathcal{T}, \mathbb{Z})$ and let $\rho : \Gamma \rightarrow \pi(\mathcal{T}) = H_1(\mathcal{T}, \mathbb{Z})$ be the isomorphism induced from η . Extend ρ to the linear isomorphism $\rho_{\mathbb{R}} : \Gamma \otimes \mathbb{R} \rightarrow H_1(\mathcal{T}, \mathbb{R})$ and get the affine isomorphism $\alpha : \Gamma \otimes \mathbb{R}/\Gamma \rightarrow H_1(\mathcal{T}, \mathbb{R})/H_1(\mathcal{T}, \mathbb{Z}) = \mathcal{T}$. Since $\rho_{\mathbb{R}} \circ \tilde{\Phi}^\Gamma$ is a lift of $\alpha \circ \Phi^\Gamma$ and

$$(53) \quad \rho_{\mathbb{R}}(\tilde{\Phi}^\Gamma(\sigma x)) = \rho_{\mathbb{R}}(\tilde{\Phi}^\Gamma(x)) + \rho(\sigma),$$

we observe that $\alpha \circ \Phi^\Gamma$ is in C . □

Put $\Phi_0 = \alpha \circ \Phi^\Gamma$ and $g_0 = c(\alpha^*)^{-1}g_{alb}$, where c is a positive constant with $v_0 = \text{vol}(cg_{alb})$. Then, for a piecewise smooth map $\Phi \in C$ and a flat metric g on \mathcal{T} with $\text{vol}(g) = v_0$, we have

$$(54) \quad \begin{aligned} E(\Phi, g) &= E(\alpha^{-1} \circ \Phi, \alpha^*g) \\ &\geq E(\Phi^\Gamma, \alpha^*g) \geq E(\Phi^\Gamma, cg_{alb}) = E(\Phi_0, g_0). \end{aligned}$$

The equality holds if and only if $g = g_0$ and Φ is a translation of Φ_0 . This completes the proof of Theorem 2, which is restated as follows:

Theorem 4.6. *Let X_0 be a finite connected weighted graph, \mathcal{T} a torus, and C a homotopy class of piecewise smooth maps from X_0 into \mathcal{T} such that a map in C induces a surjective homomorphism η of $\pi_1(X_0)$ onto $\pi_1(\mathcal{T})$. For a given positive constant v_0 , there exists a pair (Φ_0, g_0) , consisting of a harmonic map $\Phi_0 \in C$ and a flat metric g_0 on \mathcal{T} such that $\text{vol}(\mathcal{T}, g_0) = v_0$, satisfying*

$$(55) \quad E(\Phi_0, g_0) \leq E(\Phi, g)$$

for every $\Phi \in C$ and every flat metric g on \mathcal{T} with $\text{vol}(\mathcal{T}, g) = v_0$. The pair (Φ_0, g_0) coincides essentially with the pair consisting of the Albanese map and the Albanese metric associated with the Γ -crystal lattice $X = \text{Ker } \eta \backslash \tilde{X}_0$, where \tilde{X}_0 is the universal covering graph of X_0 .

Remark. It should be noted that the standard realization is not always a faithful expression of a given crystal lattice, although many examples indicate that it usually is, as will be seen in the next section. Actually if $\omega(e) = 0$ for all $\omega \in H^1(X_0, \mathbb{R})$, then the edge e degenerates in the standard realization of the maximal abelian covering graph X of X_0 , and vice versa. We call such an edge *degenerate*. Observe that an edge e is degenerate if and only if the graph obtained from X_0 by removing e is not connected. This follows from the fact that there is a circuit in X_0 which contains an edge e if and only if the graph obtained by removing e is connected. The union of all the degenerate edges forms a *forest*, a disjoint union of trees, in X . By collapsing each component of the complement of the forest in X_0 to one point, we have a tree.

5. EXAMPLES

Let us take a look at some of the classically known examples of crystal lattices. We shall see that the equilibrium configurations of those crystal lattices are just as described in their figures (Figure 2, 3, 4, 5). To explain this, we keep the notation in the previous section. We shall realize a crystal lattice X in the subspace $\Pi = (\text{Ker } \rho)^\perp$, which is identified with $\Gamma \otimes \mathbb{R}$, of the Euclidean space $H_1(X_0, \mathbb{R}) \cong \mathbb{R}^n$. Throughout this section we assume $m_V \equiv 1$ and $m_E \equiv 1$.

We shall first explain a general algorithm to realize a generalized lattice X in the Euclidean space Π . For this, take a maximal tree $T = (V_T, E_T)$ of X_0 . Fix a base point $x_0 \in T$. Then one can equip an orientation $E_0^o = \{e_1, \dots, e_n, t_1, \dots, t_{N-1}\}$ with

$$(56) \quad \begin{aligned} e_1, \dots, e_n &\notin E_T, \\ t_1, \dots, t_{N-1} &\in E_T, \end{aligned}$$

such that, for every vertex x in X_0 , there exists a minimal path $c = (t_{i_1}, \dots, t_{i_a})$ in T with $o(c) = x_0$ and $t(c) = x$. Let c_1, \dots, c_n be the basis of $H_1(X_0, \mathbb{R})$ constructed in the proof of Lemma 4.2. Take a basis $\mathbf{c}_1, \dots, \mathbf{c}_n$ of \mathbb{R}^n such that $\langle \mathbf{c}_i, \mathbf{c}_j \rangle_{\mathbb{R}^n} = \Lambda_{ij} = c_i \cdot c_j$. By identifying \mathbf{c}_i with c_i , we have an isometry between \mathbb{R}^n and $H_1(X_0, \mathbb{R})$. The vectors \mathbf{c}'_i are the orthogonal projections of \mathbf{c}_i to the k -dimensional subspace Π ($k = \text{rank } \Gamma$). Put

$$(57) \quad \mathbf{b}_i = \sum_{l=1}^n u_l(t_i) \mathbf{c}'_l \in \Pi \quad (i = 1, \dots, N-1).$$

Then we easily see that \mathbf{b}_i corresponds to $d\tilde{\Phi}^\Gamma(t_i) \in \Gamma \otimes \mathbb{R}$ through the isometry between Π and $\Gamma \otimes \mathbb{R}$.

Let $\tilde{T} \subset X$ be a lift of T , and let $\tilde{x}_0 \in \tilde{T}$ be the vertex with $\varphi(\tilde{x}_0) = x_0$. Taking the path c joining x_0 and $x = \varphi(\tilde{x})$ as above, we find that

$$(58) \quad \tilde{\Phi}^\Gamma(\tilde{x}) = \sum_{s=1}^a \mathbf{b}_{i_s} \quad (\tilde{\Phi}^\Gamma(\tilde{x}_0) = \mathbf{o}).$$

In this way, we obtain the position vectors in Π corresponding to the vertices in \tilde{T} . We draw the line segments joining two points according to the incidence of vertices and edges in \tilde{T} .

Put

$$(59) \quad \mathbf{b}_{N-1+i} = \mathbf{c}'_i - \sum_{l=1}^{N-1} f_{i,n+l} \mathbf{b}_l \quad (i = 1, \dots, n),$$

where we should recall that

$$(60) \quad c_i = e_i + \sum_{l=1}^{N-1} f_{i,n+l} t_l.$$

Therefore \mathbf{b}_{N-1+i} gives the vector in Π corresponding to $d\tilde{\Phi}^\Gamma(e_i)$. Let \tilde{e}_i be the lift of e_i with $o(\tilde{e}_i) \in \tilde{T}$. Then the figure consisting of the line segments joining $\tilde{\Phi}^\Gamma(o(\tilde{e}_i))$ and $\tilde{\Phi}^\Gamma(o(\tilde{e}_i)) + \mathbf{b}_{N-1+i}$ together with the above figure yields a building block for the standard realization. Owing to the periodicity, the realization of X is the union of its copies obtained by translations by $\mathbb{Z}\mathbf{c}'_1 + \dots + \mathbb{Z}\mathbf{c}'_n$.

Example 5.1 (The standard lattice and the triangular lattice). The standard realization of the standard lattice is the hypercubic lattice (Figure 2), and that of the triangular lattice is the equilateral triangular lattice (Figure 3.a). Note that Figure 3.b gives a crystal lattice whose internal force is in equilibrium but where configuration is not.

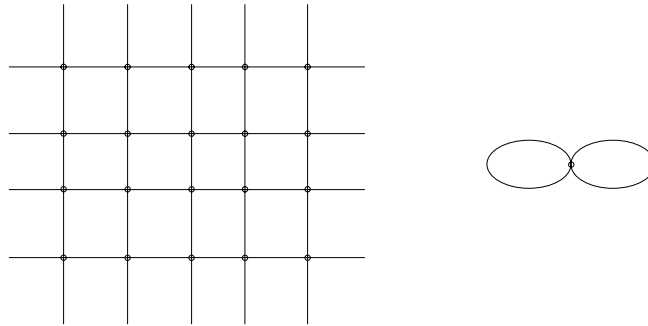


FIGURE 2. The standard lattice and its quotient graph

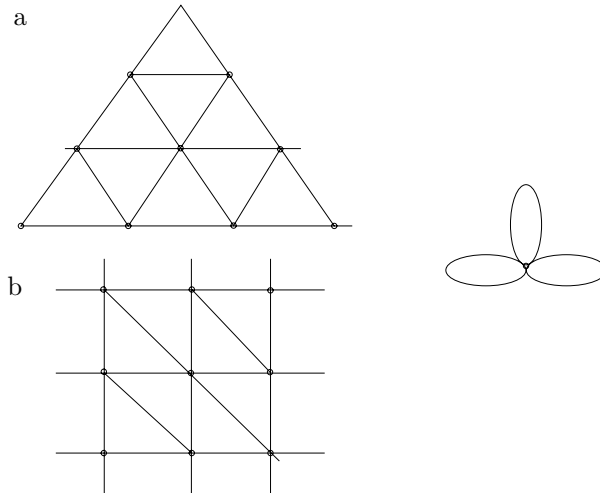


FIGURE 3. The triangular lattice (with equilibrium configuration and non equilibrium configuration)

Example 5.2 (The n -diamond lattice). Consider the maximal abelian covering graph X_0^{ab} of the graph X_0 with two vertices joined by $n + 1$ multiple edges e_1, \dots, e_{n+1} (Figure 1). Put $c_i = e_i \bar{e}_{n+1}$ for $i = 1, \dots, n$, which forms a \mathbb{Z} -basis of $H_1(X_0, \mathbb{Z})$. We have

$$F = \left(\begin{array}{cccc|c} 1 & 0 & \cdots & 0 & -1 \\ 0 & 1 & \cdots & 0 & -1 \\ \vdots & & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -1 \end{array} \right),$$

$$\Lambda = \begin{pmatrix} 2 & 1 & \cdots & 1 \\ 1 & 2 & \cdots & 1 \\ \vdots & & \ddots & \vdots \\ 1 & 1 & \cdots & 2 \end{pmatrix}, \quad U = \frac{1}{n+1} \begin{pmatrix} n & -1 & \cdots & -1 \\ -1 & n & \cdots & -1 \\ \vdots & & \ddots & \vdots \\ -1 & -1 & \cdots & n \end{pmatrix}.$$

Therefore

$$(61) \quad \begin{aligned} \mathbf{b}_i &= \mathbf{c}_i - \frac{1}{n+1} \sum_{l=1}^n \mathbf{c}_l \quad \text{for } i = 1, \dots, n, \\ \mathbf{b}_{n+1} &= \frac{-1}{n+1} \sum_{l=1}^n \mathbf{c}_l. \end{aligned}$$

Then we find that $\langle \mathbf{b}_i, \mathbf{b}_j \rangle = \delta_{ij} - \frac{1}{n+1}$. The realization of X_0^{ab} is the figures consisting of $n+1$ vertices \mathbf{b}_i of an equilateral $(n+1)$ -simplex joined by line segments with the center of mass at the origin and its copies obtained by translation by $\sum_{i=1}^n \mathbb{Z}\mathbf{c}_i$. It is now easy to see that the n -diamond lattice graph is the hexagonal lattice graph when $n=2$ (Figure 4), and it gives the crystal structure of diamond when $n=3$.

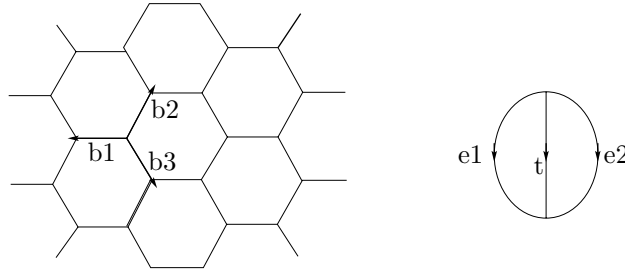


FIGURE 4. The hexagonal lattice and its quotient graph

Example 5.3 (The Kagome lattice). The Kagome lattice is the \mathbb{Z}^2 -crystal lattice with the quotient graph X_0 which consists of three vertices joined by double edges (see Figure 5). Put $c_1 = e_1 \bar{t}_1$, $c_2 = e_2 \bar{t}_2$, $c_3 = t_1 e_3 \bar{t}_2$, $c_4 = t_1 e_4 \bar{t}_2$, which form a \mathbb{Z} -basis of $H_1(X_0, \mathbb{Z})$. Here we realize first the maximal abelian covering graph X_0^{ab} of X_0 and then the Kagome lattice as the image of the orthogonal projection of the realization of X_0^{ab} to the 2-dimensional subspace $\Pi = \text{Ker } \rho^\perp$.

We have

$$F = \left(\begin{array}{cccc|cc} 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 & 1 & -1 \end{array} \right),$$

$$\Lambda = \begin{pmatrix} 2 & 0 & -1 & -1 \\ 0 & 2 & 1 & 1 \\ -1 & 1 & 3 & 2 \\ -1 & 1 & 2 & 3 \end{pmatrix}, \quad U = \frac{1}{6} \begin{pmatrix} 4 & -1 & 1 & -1 \\ -1 & 4 & -1 & -1 \\ 1 & -1 & 4 & -2 \\ 1 & -1 & -2 & 4 \end{pmatrix}.$$

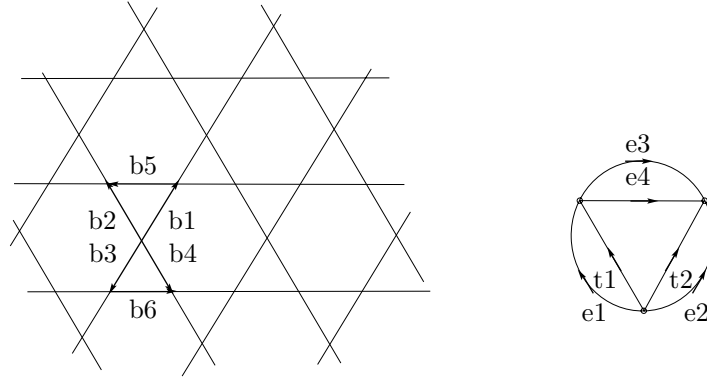


FIGURE 5. The Kagome lattice and its quotient graph

1) The maximal abelian covering graph X_0^{ab} ($n = k = 4$).

Let $\mathbf{c}_i \in \mathbb{R}^4$ be the vector corresponding to c_i for $i = 1, 2, 3, 4$, so that $((\mathbf{c}_i, \mathbf{c}_j)_{\mathbb{R}^4}) = \Lambda$. By simple computation, we have

$$(62) \quad \mathbf{b}_1 = \frac{1}{6}(-2\mathbf{c}_1 - \mathbf{c}_2 + \mathbf{c}_3 + \mathbf{c}_4),$$

$$(63) \quad \mathbf{b}_2 = \frac{1}{6}(-\mathbf{c}_1 - 2\mathbf{c}_2 - \mathbf{c}_3 - \mathbf{c}_4),$$

$$(64) \quad \mathbf{b}_3 = \frac{1}{6}(4\mathbf{c}_1 - \mathbf{c}_2 + \mathbf{c}_3 + \mathbf{c}_4),$$

$$(65) \quad \mathbf{b}_4 = \frac{1}{6}(-\mathbf{c}_1 + 4\mathbf{c}_2 - \mathbf{c}_3 - \mathbf{c}_4).$$

The building block of the realization of X_0^{ab} consists of the two triangles $\Delta\mathbf{ob}_1\mathbf{b}_2$ and $\Delta\mathbf{ob}_3\mathbf{b}_4$, and the realization of X_0^{ab} is the union of their copies obtained by translation by $\sum \mathbb{Z}\mathbf{c}_i$.

2) The Kagome lattice ($n = 4, k = 2$).

A basis of Γ is given by $\rho(c_1) = \sigma_1$ and $\rho(c_2) = \sigma_2$. Since $\rho(c_4) = 0$ and $\rho(c_3) = \sigma_2 - \sigma_1$, $\text{Ker } \rho = \text{Span}\{c_4, c_1 - c_2 + c_3\}$. The Kagome lattice is realized in the subspace $\Pi = \text{Ker } \rho^\perp \subset \mathbb{R}^4$, and the action of Γ is generated by translation of the orthogonal projection \mathbf{c}'_i of \mathbf{c}_i for $i = 1, 2$ to the subspace Π . The orthogonal projection of \mathbf{b}_i in (1) to Π gives the realization of the vertices of the building block of the Kagome lattice in Π , which we also denote by \mathbf{b}_i . They are given by

$$(66) \quad \mathbf{b}_1 = v_1(t_1)\mathbf{c}'_1 + v_2(t_1)\mathbf{c}'_2 = -\frac{1}{2}\mathbf{c}'_1,$$

$$(67) \quad \mathbf{b}_2 = v_1(t_2)\mathbf{c}'_1 + v_2(t_2)\mathbf{c}'_2 = -\frac{1}{2}\mathbf{c}'_2,$$

$$(68) \quad \mathbf{b}_3 = \mathbf{c}'_1 + \tilde{\Phi}(p_1) - \tilde{\Phi}(o) = \frac{1}{2}\mathbf{c}'_1,$$

$$(69) \quad \mathbf{b}_4 = \mathbf{c}'_2 + \tilde{\Phi}(p_2) - \tilde{\Phi}(o) = \frac{1}{2}\mathbf{c}'_2.$$

By using the relations

$\langle \cdot, \cdot \rangle$	c_4	c_1	c_2	$c_1 - c_2 + c_3$
c_4	3	-1	1	0
c_1	-1	2	0	1
c_2	1	0	2	-1
$c_1 - c_2 + c_3$	0	1	-1	3

we have

$$\begin{aligned}
 (70) \quad \mathbf{c}'_1 &= \mathbf{c}_1 - \frac{1}{3} \langle \mathbf{c}_1, \mathbf{c}_1 - \mathbf{c}_2 + \mathbf{c}_3 \rangle (\mathbf{c}_1 - \mathbf{c}_2 + \mathbf{c}_3) - \frac{1}{3} \langle \mathbf{c}_1, \mathbf{c}_4 \rangle \mathbf{c}_4 \\
 &= \frac{1}{3} (2\mathbf{c}_1 + \mathbf{c}_2 - \mathbf{c}_3 + \mathbf{c}_4),
 \end{aligned}$$

$$\begin{aligned}
 (71) \quad \mathbf{c}'_2 &= \mathbf{c}_2 - \frac{1}{3} \langle \mathbf{c}_2, \mathbf{c}_1 - \mathbf{c}_2 + \mathbf{c}_3 \rangle (\mathbf{c}_1 - \mathbf{c}_2 + \mathbf{c}_3) - \frac{1}{3} \langle \mathbf{c}_2, \mathbf{c}_4 \rangle \mathbf{c}_4 \\
 &= \frac{1}{3} (\mathbf{c}_1 + 2\mathbf{c}_2 + \mathbf{c}_3 - \mathbf{c}_4).
 \end{aligned}$$

Notice that $\triangle \mathbf{oc}'_1 \mathbf{c}'_2$ forms an equilateral triangle with edges of length $2/\sqrt{3}$. The building block of the realization of the Kagome lattice consists of the two triangles $\frac{1}{2} \triangle \mathbf{oc}'_1 \mathbf{c}'_2$ and $\frac{-1}{2} \triangle \mathbf{oc}'_1 \mathbf{c}'_2$, and the realization of the Kagome lattice is the union of their copies obtained by translation by $\mathbb{Z}\mathbf{c}'_1 + \mathbb{Z}\mathbf{c}'_2$ in the subspace Π .

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