Displacive transformations and quasicrystalline symmetries

Michel Duneau, Christophe Oguey

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Displacive transformations and quasicrystalline symmetries

Michel Duneau and Christophe Oguey

Centre de Physique Théorique, Ecole Polytechnique, F-91128 Palaiseau Cedex, France

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Résumé. — La propriété, pour une structure quasi-périodique obtenue par coupe et projection ou toute autre méthode équivalente, d'être liée à un réseau moyen par une déformation bornée est une forte restriction sur la fenêtre définissant la bande, ou sur la surface atomique. Nous donnons une condition suffisante (nécessaire à une dimension) pour l'existence d'une telle modulation vers un réseau, qui stipule que la fenêtre pave l'espace orthogonal. Grâce à une construction spéciale nous étendons notre preuve à des situations plus générales, bien que non génériques, incluant les pavages du type Penrose.

Abstract. — The property, for quasiperiodic structures built by the cut and project or any equivalent method, to be related to a periodic lattice by a bounded deformation is a strong restriction on the window defining the strip, or on the atomic surface. We give a sufficient condition (which is also necessary in one dimension) for the existence of such a bounded modulation to a lattice which requires that the window tiles the orthogonal space. Using a special procedure we extend our proof to more general, albeit still non generic, situations including tilings of the Penrose type.

1. Introduction.

Generalising the definitions of quasiperiodic functions [1], affine sections of periodic structures in higher dimensions provide quasiperiodic patterns in the Euclidean space. As such, they provide suitable templates to account for the atomic ordering in modulated crystals and quasicrystals. For example, using the section method in 6 dimensions [2, 3], one can build discrete sets of atomic sites with a pure point Fourier spectrum and icosahedral point symmetry similar to the icosahedral phases of AlMnSi [4] or AlFeCu [5] alloys. Once the quasi-periodicity is ensured and the symmetry constraints are satisfied, the 3-dimensional patterns only depend on the shape and positions of the atomic surfaces — the codimension 3 surfaces providing the atomic sites by intersection with the physical space — in the 6-dimensional unit cell. Although some models give reasonable fits for the Ico-AlMnSi phase, the determination of the atomic surfaces cannot yet be considered as definitively solved.

In many cases, the quasicrystalline phases are obtained by fast quenching from the liquid phase ; under annealing or spontaneous « ageing » at room temperature, a transition to neighboring crystalline phases is often observed [6]. In other alloys such as the AlFeCu, the quasicrystalline phase is believed to be a stable thermodynamic state. In this case the coexistence of a quasicrystal and crystalline phase refers to a true first order phase transition.

The present paper is devoted to transitions of the *displacive* type. By this we mean that the change of the atomic positions, from one phase to the other, is described by local — bounded — displacements of the atoms throughout the whole bulk material. In particular, such transitions preserve the densities and concentrations. On the opposite, phase transitions involving changes in, say, concentrations are of the *diffusive* type and imply atomic migrations at a macroscopic scale (the scale of the monocrystalline grains). For example, the Ico-α transition in the AlMnSi alloy is diffusive whereas the Ico-β transition might be of the displacive type.

When the displacements are given by a periodic or quasiperiodic function, we speak of a *modulation*. Modulated crystals are indeed characterized by a *reference* lattice — the « unmodulated » lattice, which may or not be the Bravais lattice of an existing solid state of the alloy — and a modulation inferred from the « satellite » spots in the diffraction patterns. Modulated crystals may as well be described as affine sections of a periodic set of « atomic surfaces » in $n = d + d'$ dimensions, d being the dimension of the physical space, d' the dimension of the frequency module of the hull function ($d' \leqslant d$ if it is a periodic function) [7].

Another set of examples is provided by the quasiperiodic tilings ; because of the finite number of local patterns — which is conjectured to correspond to a similar finiteness in the local atomic configurations —, the « atomic surfaces » look like a collection of bounded disconnected pieces with boundaries [8-12]. As in the case of modulated crystals, the higher dimension n is equal to (or larger than) the number of basis vectors necessary to index the diffraction spectrum, and the lattice parameters as well as the direction of the cut with respect to the lattice are fixed, up to trivial equivalences [3, 7], by the coordinates of the diffraction spots (this determination being greatly simplified by the high order point symmetries observed in quasicrystals).

The very existence of a displacement which maps the quasiperiodic structure onto a periodic one is already a non trivial statement. It may happen that 1) there exists no reference lattice related to the quasiperiodic pattern by bounded displacements ; 2) in the cases where such a map exists, the displacements may not be a modulation (the existence of a modulation function being forbidden by topological obstruction).

Indeed, in the cut and project algorithms, if we choose and fix the direction of the cut, the existence of a reference lattice — together with the displacement map — is a *non generic* property of the profile of the strip or of the atomic surface in $E^{\perp}$. The purpose of the present paper is to provide a set of instances — in arbitrary dimension — where such a displacive transform to a lattice is actually possible, and to give its explicit construction.

The non-genericity of the existence of the reference lattice was put to evidence in 1D tilings generated by the multiples modulo 1 of an irrational number (the « circle map » algorithm) [13]. Such statements go back to a theorem of Kesten in number theory [14]. In 1D, the parameter of the candidate « average lattice » is uniquely provided by the inverse of the density. From the connection between the circle map and the cut and project method in the lowest dimension it is straightforward to deduce that 1D quasiperiodic tilings admit an average lattice if and only if the width of the strip is a (2D) lattice vector.

In higher dimensions, tentatives to build quasiperiodic tilings by superposition of modulated crystals were investigated by Spal [15] and by Kalugin *et al.* [16]. With our results, a global reference lattice can be constructed for those models.

Formal definitions and a few notations are given in section 2.

Qualitatively, the argument in section 3 is the following. In previous tentatives to approximate the quasicrystalline phase by periodic phases, the approximants were obtained by a slight tilt of the *section* space (of the strip in the cut and project method) so as to give it a rational orientation w.r.t. the lattice Λ. A different procedure keeps the section (strip) fixed, but changes the *atomic surface* within a torus (equivalently : the kernel of the projector p) so

that $E' = \text{Ker}\ (p)$ becomes a lattice plane. This last method has received little attention (see however Gratias [17]). A plausible reason is that if, on one hand, the projected lattice $L = p(\Lambda)$ is indeed a lattice in the physical space (isomorphic to the quotient Λ/L'_r by $L'_r = \Lambda \cap \text{Ker}\ (p)$), on the other hand, the pattern X^r is *in general* nothing more than *a quasiperiodic subset* of L. The only cases where this subset is periodic — counting degenerate projections as coinciding atoms, a situation forbidden from the physical point of view — is when X^r coincides with L ; this yields the « cell » constraint we state in theorem 3.1 to get a reference lattice.

In section 4, the existence of a map to a crystal is shown to hold true for quasiperiodic patterns which are superpositions — in a way analogous to an « inter-growth » [18] — of patterns of the type considered in the previous section. This extended class contains all cases of interest for crystallography. In particular, the set of vertices of the octagonal, icosahedral or Penrose type tilings do map to a lattice in a one to one way. A central Lemma on displacements between lattices with the same density is used in section 4 buts its proof and discussion are postponed to section 5.

What is concerned in this paper is the geometrical map from an atomic structure to another. Of course this map need not represent the real motion of the atoms during the possible transition. Nor do we carry out the quantitative analysis (eventually) leading to an *optimal* set of displacements (w.r.t. energetic or geometric criteria). Current work is in progress in this area. To us, the surprise is that even such a weak condition as the mere existence of the displacement — regardless of its detailed effect onto the local atomic ordering — provides non-trivial (and actually severe) conclusions as to the atomic surfaces.

2. Definitions and settings.

Let X be a discrete subset of $\mathbb{R}^d$ such as the set of atomic sites in a condensed matter phase. A *displacive map* is an injective [1] map f: $X \to \mathbb{R}^d$ which is uniformly bounded in the following sense : there is a finite constant $c > 0$ such that $\| f(x) - x \| \leqslant c$ for all x of X. The proper *displacement* $\delta(x) = f(x) - x$ is a uniformly bounded « vector field » on X.

The possible extension of f to a one to one, piecewise continuous, mapping of $\mathbb{R}^d$ is not required in our definition but will be actually ensured by our construction.
Let $Y = f(X)$. Then the map f: $X \leftrightarrow Y$ is one to one ; it is the displacement from X to Y. Given such a displacement f, the *f-distance* between X and $Y = f(X)$ is the length of the largest displacement vector in the field : $\sup_{x \in X} \| f(x) - x \|$. We also speak of the *distance* between two discrete patterns X and Y as the smallest f-distance over all possible displacements f from X to Y :

$$d(X, Y) = \inf_{f : X \leftrightarrow Y} \sup_{x \in X} \| f(x) - x \| .$$

When there is no displacement between X and Y we set $d(X, Y) = \infty$.

Let E (the physical space) be a d-dimensional subspace of $\mathbb{R}^n$ $(0 < d < n)$ and let E' be a $(n - d)$-dimensional complement of E. Denote p and p' the two complementary projectors onto E (with kernel E') and E' (with kernel E).

$$\begin{aligned} E &= p(\mathbb{R}^n) \\ E' &= p'(\mathbb{R}^n) \\ \mathbb{R}^n &= E \oplus E' . \end{aligned}$$

[1] The map is injective if $f(x) \neq f(x')$ for any $x \neq x'$.

Let Λ be a n-dimensional lattice in $\mathbb{R}^n$ generated by the basis $\{a_1, \ldots, a_n\}$.

$$\Lambda = \left\{ \sum_{i=1}^{n} z_i \quad a_i \,|\, z_i \in \mathbb{Z} \text{ for } i = 1, \ldots, n \right\} = [a_1, \ldots, a_n] .$$

The projections of the lattice Λ into E and E' are $\mathbb{Z}$-modules L and L' given by :

$$\mathrm{L} = p(\Lambda) = \left\{ \sum_{i=1}^{n} z_i \quad e_i \,|\, z_i \in \mathbb{Z} \text{ for } i = 1, \ldots, n \right\}$$

with $e_i = p(a_i)$ for $i = 1, \ldots, n$.

$$\mathrm{L}' = p'(\Lambda) = \left\{ \sum_{i=1}^{n} z_i \quad e_i' \,|\, z_i \in \mathbb{Z} \text{ for } i = 1, \ldots, n \right\}$$

with $e_i' = p'(a_i)$ for $i = 1, \ldots, n$.
Once the orientation of the physical space E in $\mathbb{R}^n$ is given (for instance by symmetry requirements) an important parameter of the construction is the relative translation between E and the lattice Λ (leading to the « phason modes »). For simplicity we assume that the physical space E is fixed (together with the strip) and that the lattice Λ undergoes this translation : For any given τ in $\mathbb{R}^n$ define

$$\begin{aligned} \Lambda_\tau &= \Lambda + \tau . \\ \mathrm{L}_\tau &= p(\Lambda_\tau) = \mathrm{L} + t , \qquad \text{where } t = p(\tau) \\ \mathrm{L}'_\tau &= p'(\Lambda_\tau) = \mathrm{L}' + t' , \quad \text{where } t' = p'(\tau) . \end{aligned}$$

Assume W is a bounded open subset of E' and define the corresponding « strip » by

$$\mathrm{S} = \mathrm{E} \times \mathrm{W} = \{ x + x' \,|\, x \in \mathrm{E} \text{ and } x' \in \mathrm{W} \} .$$

The cut and project method starts by selecting the set Ξ_τ of lattice nodes which belong to the strip :

$$\Xi_\tau = \Lambda_\tau \cap \mathrm{S} .$$

Then this subset is projected onto E, yielding a d-dimensional Delaunay set X_τ :

$$\mathrm{X}_\tau = p(\Xi_\tau) = p(\Lambda_\tau \cap \mathrm{S}) .$$

If the window W and the translation τ are such that the boundary ∂W of W does not meet L'_τ then X_τ is a regular quasiperiodic pattern. When τ runs through a fundamental domain of Λ in $\mathbb{R}^n$ the various X_τ form a class of equivalent tilings of patterns ([2]).

3. Modulations.

In this section we describe quasiperiodic patterns which are basically equivalent to modulated crystals. The displacements involved here are (eventually discontinuous) periodic or quasiperiodic vector fields which we call modulations.

THEOREM 3.1. — If W is a unit cell of a certain $(n - d)$-dimensional lattice L'_0 contained in L' then the above defined structure X_τ may be mapped onto a lattice by a modulation.

([2]) This is true only when E is completely irrational in Λ.

Proof:

Since L'_0 is a sublattice of L', there exists a $(n-d)$-dimensional sublattice Λ_0 of Λ such that $L'_0 = p'(\Lambda_0)$. Let E_0 be the subspace spanned by Λ_0 and let Ω denote the intersection of E_0 with the strip S : $\Omega = E_0 \cap S$ (see Fig. 1). Thus :

$$L'_0 = p'(\Lambda_0)$$
$$W = p'(\Omega)$$

where, by hypothesis, Ω is a unit cell for Λ_0. The strip S has the equivalent definition

$$S = E \times \Omega = \{x + y \,|\, x \in E \text{ and } y \in \Omega\} .$$

Now Λ_0 is a sublattice of the intersection lattice $\Lambda \cap E_0$. We consider two cases according to whether Λ_0 is equal to, or strictly included in, $\Lambda \cap E_0$.

Case 1 : $\Lambda_0 = \Lambda \cap E_0$.

By elementary linear algebra, there exists a complementary sublattice Λ_1, spanning a subspace E_1, such that we have the direct sums (see [19]) :

$$\Lambda = \Lambda_0 \oplus \Lambda_1$$
$$\mathbb{R}^n = E_0 \oplus E_1 .$$

Define π as the oblique projector with range E and kernel E_0.

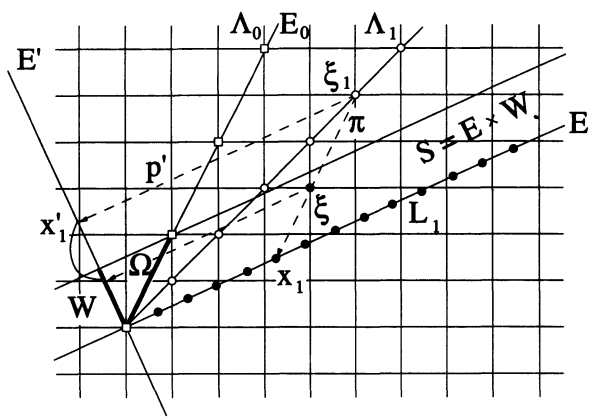

Fig. 1. — The window W is the projection of a fundamental cell Ω of the sublattice Λ_0 which spans the vector space E_0 ; Λ_1 is a complement of Λ_0. The oblique projection π maps the lattice Λ_1 onto L_1 in the physical space E. The vertex ξ gives the orthogonal projection x in the quasiperiodic structure, and $x_1 = \pi(\xi)$ in the reference lattice.

We claim that a mean lattice for X_τ is given, up to a translation, by the oblique projection of Λ_1 onto E :

$$L_1 = \pi(\Lambda) = \pi(\Lambda_1) .$$

Indeed the oblique projection π provides a one to one mapping between Ξ_τ and $\pi(\Lambda_1 + \tau) = L_1 + t_1$ where $t_1 = \pi(\tau)$:

i) Since $\Xi_\tau \subset \Lambda_\tau$ we have the inclusion $\pi(\Xi_\tau) \subset \pi(\Lambda_\tau) = L_1 + t_1$.

ii) On the other hand, for any x_1 in $L_1 + t_1$ there exists a point ξ_1 of Λ_τ such that $x_1 = \pi(\xi_1) = \pi(E_0 + \xi_1)$ (see Fig. 1). By hypothesis the $(n-p)$-plane $E_0 + \xi_1$ has an

intersection with the strip S which is a unit cell for the translated lattice $\Lambda_0 + \xi_1$ and therefore $(E_0 + \xi_1) \cap S$ contains a unique lattice node ξ ; this point ξ belongs to the set Ξ_τ and satisfies $\pi(\xi) = x_1$.

Now, the one to one bounded mapping between X_τ and $L_1 + t_1$ is easily obtained in the following way : for any point ξ which belongs to Ξ_τ we consider the projection $x = p(\xi)$ in X_τ and $x_1 = \pi(\xi)$ in $L_1 + t_1$; the mapping ϕ is defined by $\phi(x) = x_1$. An upper bound C for the distances $\|x - \phi(x)\|$ follows merely from the assumption that W, and therefore Ω, are bounded.

Case 2 : $\Lambda_0 \neq \Lambda \cap E_0$.

In this case, Λ_0 is a sublattice of $\Lambda \cap E_0$ and there is a basis B (a finite set of points) such that

$$\Lambda_0 + B = \Lambda \cap E_0 .$$

Define Λ_1 as a complement of $\Lambda \cap E_0$ in Λ. The construction is similar to case 1. The only difference is that the oblique projection $\pi(\Xi_\tau)$ of Ξ_τ onto $L_1 + t_1$ is no more injective ; actually, for any point x_1 in $L_1 + t_1$ there exists a point η in Ξ_τ such that $B + \eta$ is the intersection of the lattice $\Lambda_0 + \eta$ with the strip S ; consequently, $x_1 = \pi(B + \eta)$. In other words $\Xi_\tau = H_\tau \oplus B$; H_τ is the set of vertices selected by a window Ω which is a fundamental domain of $\Lambda \cap E_0$, as in case 1.

Now map B into E in an injective way ($B \to B_1 \subset E$; for ex. $B_1 = p(B)$). Then Ξ_τ is in 1-1 bounded correspondence with the periodic set $L_1 + B_1$ — a lattice with a structural basis —.

Remarks :

— In the proof a global translation of L_1 can be used in order to decrease the constant C ; ϕ is simply defined by $\phi(x) = x_1 - t_1 + s$ where s is a vector in E ; similarly the basis B_1 can be optimized.

— In the proof, the upper bound C is of the order of the diameter of Ω. In most cases this is far from optimal. Better bounds can be found by « relabelling » the atoms, that is, changing the relation $f: X \leftrightarrow Y$ without changing the positions of the vertices in either X or Y [13]. This relabelling causes the task of getting tight estimates of the displacements delicate.

SIMPLE APPLICATIONS.

a) *Canonical 1D quasiperiodic tilings.* — Consider the case where $d = 1$. The physical space E is generated by a vector u :

$$u = \sum_{i=1}^{n} u_i \quad a_i$$

and we can assume that $\sum_{i=1}^{n} |u_i| = 1$.

E is supposed to be completely irrational w.r.t. the lattice Λ ; in particular all the coordinates u_i are different from 0. E′ is the hyperplane orthogonal to E and the strip is $E \times W$ where W is the projection $p'(\gamma)$ of the unit cube γ of the lattice Λ.

We first show :

LEMMA 3.2. — W is the unit cell of a $(n-1)$-dimensional lattice $L'_0 \subset L'$.
(Notice that for $n = 3$ W is a hexagon and for $n = 4$ W is a rhombic dodecahedron).

Proof :

W is the zonohedron $Z(e'_1, \ldots, e'_n)$ spanned by the n vectors $e'_i = p'(a_i)$; the boundary of W is

made of zonohedra $Z_{ij}(e'_1, \ldots, e'_n)$ where e'_i, e'_j are omitted (these are the $(n-2)$-dimensional facets of W) which are translated either by 0 and $e'_i + e'_j$, or by e'_i and e'_j (this is easily seen in the 2-plane generated by $\{e'_i, e'_j\}$) ; the first case corresponds to 0 being on the boundary of W whereas the second case corresponds to 0 being an interior point of W. After possibly changing some signs in the definition of the basis $\{a_1, \ldots, a_n\}$ we can assume that all coordinates u_i of u are positive ; this implies that 0 is an interior point of W and consequently that the facets of W are congruent modulo $(e'_i - e'_j)$. These $n(n-1)$ vectors span a $(n-1)$-dimensional lattice L'_0 a basis of which is given for instance by the $n-1$ vectors $e'_i - e'_n$ for $i = 1, \ldots, n-1$.

COROLLARY 3.3. — In these $d = 1$ settings, the mean lattice is Zu.

Proof:

For a generic translation τ (see the discussion of the general case) the corresponding one-dimensional quasiperiodic structure is $X_\tau = p(\Lambda_\tau \cap S)$. In the notations of the lemma, L'_0 is the projection of the lattice Λ_0 generated by $\{a_i - a_n \mid i = 1, \ldots, n-1\}$ and Λ_0 spans a hyperplane E_0. A complement of Λ_0 is for instance the one-dimensional lattice $\Lambda_1 = \mathbb{Z} \cdot a_n$ generated by a_n. Following the above procedure we obtain the mean lattice of X_τ as the oblique projection $\pi(\Lambda_1)$ onto E where π is the projector of range E and kernel E_0. The mean lattice $L_1 = \pi(\Lambda_1)$ is generated by $\pi(a_n)$ and since $u = \sum_{i=1} u_i \cdot (a_i - a_n) + a_n$ it is easily checked that $\pi(a_n) = u$.

b) *Codimension 1 systems.* — When $d = n - 1$ the strip is a slice whose profile along the line E′ is a segment.

COROLLARY 3.4. — If the width of the strip is a vector of the module L′, then there exists a d-dimensional lattice at bounded distance from X_τ.

Proof:

Let $x' \in L'$ be the width of S. The interval $[0, x')$ is a cell for the sublattice $L'_0 = Z \cdot x'$ of L′. The theorem concludes.

In particular, the $(n-1)$ D canonical tilings can be mapped onto a lattice by a modulation ([3]) since, once projected into E′, the unit cube γ_n coincides with one of its diagonals.

Remark. — Basically, these settings in $n = d + 1$ dimension are closely related to de Wolf-Janner-Janssen's description of modulated crystals [7]. In their method, the atomic lines are continuous and project onto closed loops in the torus T^n. Any such loop can be deformed into a basic circle which provides the lattice by section with E. The condition stated in corollary 3.4 ($|S \cap E'| \in L'$) essentially means that the atomic segment, once projected in T^n, are equivalent to closed loops ; the « horizontal » segment necessary to close the loop (joining the origin to the end of the « vertical » atomic segment) may be chosen in E, which makes it invisible in *generic* sections $E + \tau$.

4. Generalizations.

Using the results of section 3 we extend the existence of a reference lattice to more general situations. The problem reduces to the study of displacements between conventional lattices, an exercise which will be handled in the next section.

([3]) Conventionally, one would state things the other way around : the quasiperiodic pattern is a modulated lattice !

THEOREM. 4.1. — Suppose the window W is a disjoint union of cells $W_1, \ldots, W_k$, each cell W_i being a fundamental cell for a $(n-d)$-dimensional lattice L'_i contained in L'. Then X_t may be mapped onto a lattice by displacement.

Proof:

Since X_τ is in 1-1 correspondence with $W \cap L'_\tau$ in the complementary space E', the partition $W = \bigcup_i W_i$ induces a partition of X_τ into $X_\tau^{(1)}, \ldots, X_\tau^{(k)}$.

Each $X_\tau^{(i)}$ satisfies the hypothesis of theorem 3.1 so that it is related to a reference lattice L_i by a modulation. The whole set X_τ is thus related to the union $\bigcup_i L_i$ of the various lattices.

By corollary 4.3, below, this union is in turn related to a single common lattice L.

Remarks:

1. The displacement involved in this theorem is not a modulation. Different modulations apply to uniformly spread subsets of the pattern.

2. The union $\cup L_i$ is in general not a Delaunay set. It is relatively dense but satisfies no minimum distance condition. This is of no importance since this structure is only an intermediate step in the proof ; we do not pretend that the real motion of the atoms follows such a path.

LEMMA 4.2. — Let L_1, L_2 be two 1D lattices. There exists an average lattice L for the union $L_1 \cup L_2$.

Proof:

Without restriction, we may suppose $L_1 = a \cdot \mathbb{Z}$ and $L_2 = \mathbb{Z} + b$ with $0 < a \leq 1$ and $0 \leq b < 1$.

Let $x \in \mathbb{R}$. In the interval $(0, x]$ there are $n = \text{Int}\,(x/a) + \text{Int}\,(x-b)$ points of $L_1 \cup L_2$. This implies that $x_n \leq x < x_n + a$, i.e. $|x_n - x| < a$, where x_n is the n'th point of the pattern starting from 0.

On the other hand, by definition of n, $|(x/a + x) - n| \leq 3$, which implies $|x - na/(a+1)| \leq 3\,a/(a+1)$.
Gathering those bounds yields

$$|x_n - na/(a+1)| \leq |x_n - x| + |x - na/(a+1)| \leq a + 3\,a/(a+1) < 4\,. \qquad \text{QED}$$

Remark: the density of $L_1 \cup L_2$ is of course the sum of the densities $n(L_1) + n(L_2)$.

LEMMA 4.3. — Let L_1, L_2 be two n-D lattices in $\mathbb{R}^n$. Then there exists a lattice L at finite distance from $L_1 \cup L_2$.

Proof:

Let $L_1 = [a_1, \ldots, a_n]$ and $L_2 = [b_1, \ldots, b_n]$ and $n(L)$ be the density of L. Set $r = n(L_1)/n(L_2)$. The lattice $L_3 = [a_1, \ldots, a_{n-1}, r \cdot a_n]$ has the same density as L_2. So, by theorem 5.2 in the next section, there is a displacement mapping L_2 onto L_3. Define L as $L = [a_1, \ldots, a_{n-1}, r(r+1)^{-1} \cdot a_n]$. Then the end of the proof is a straightforward consequence of lemma 4.2 since L_1, L_3 and L only differ on the a_n axis. QED

Further extensions.

W can be decomposed into a disjoint union of W'_is and there exist translations t'_i in L' such that the subsets $W_i + t'_i$ are pairwise disjoint and the new window

$W' = \cup (W_i + t_i')$ satisfies the condition of Theorem 4.1. Actually, the structures defined by the windows W_i and $W_i + t_i'$ only differ by a finite translation t_i such that $\tau_i = (t_i, t_i')$ is a vertex of Λ.

Consequences.

In most of the usual examples of quasiperiodic tilings the simple condition that the window W is a unit cell is not fulfilled. For instance, the window for the octagonal tiling is an octagon whereas the window of the 3D Penrose tiling is a triacontahedron. Here the obstruction is a consequence of the symmetry requirement.

However these tilings fall into the possible extensions stated here. The case of the octagonal tiling is handled in detail in appendix 1. Concerning the 3D Penrose tiling, we can observe that the triacontahedron W splits into 10 large rhombohedra and 10 small ones. Each rhombohedron is a fundamental cell for some 3D lattice in the module L'. Actually this is a common feature of all « canonical » quasiperiodic tilings which are built by cutting a set atomic surfaces obtained as the E'-projection of a primitive cell of the lattice Λ. The projected unit cube is trivially tiled by a subset of its d'-dim. facets and these facets are primitive cells for d'-dim. sublattices of Λ.

5. Displacements in crystals !

In this section we show that if two n-dimensional lattices have the same density in $\mathbb{R}^n$ then a bounded one to one mapping between them can be constructed.

First, we need a simple result as to the profiles of primitive cells.

LEMMA 5.1. — Let

$$\Omega_a = \left\{ \sum_{i=1}^{n} x_i \quad a_i \,|\, -\frac{1}{2} \leq x_i < \frac{1}{2} \text{ for } i = 1, \ldots, n \right\}$$

and

$$\Omega_b = \left\{ \sum_{i=1}^{n} x_i \quad b_i \,|\, -\frac{1}{2} \leq x_i < \frac{1}{2} \text{ for } i = 1, \ldots, n \right\}$$

be the two centered parallelohedra generated by the basis $\{a_1, \ldots, a_n\}$, $\{b_1, \ldots, b_n\}$ respectively. Assume Ω_a and Ω_b have equal volume. Then there is a unit vector u in $\mathbb{R}^n$ such that the orthogonal projections of Ω_a and of Ω_b onto the line spanned by u are equal.

Proof:

Let K be the convex hull of the union of Ω_a and Ω_b ; K is a parallelohedron which is symmetric with respect to the origin. The vertices of K are vertices of either Ω_a or Ω_b. Moreover there is a facet with at least one vertex in those of Ω_a and another vertex in those of Ω_b (otherwise one of the cells contains the other one, which contradicts the equal volume hypothesis unless $\Omega_a = \Omega_b$). By central symmetry, a second facet of K enjoys the same property. Choose u to be perpendicular to those two facets ; the orthogonal projections of Ω_a and Ω_b (and K) onto $\mathbb{R} \cdot u$ are equal (see Fig. 2). QED

THEOREM 5.2. — Let Λ_a and Λ_b be two n-dimensional lattices in $\mathbb{R}^n$ and assume they have the same density. Then there exist a constant C and a one to one mapping f between Λ_a and Λ_b such that the distance $\|x - f(x)\| < C$ for all x in Λ_a.

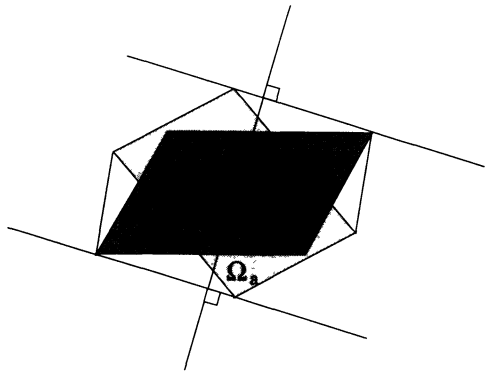

Fig. 2. — Construction of a direction u on which the two cells Ω_a and Ω_b, of equal volume, have the same projection.

Proof:

Suppose $\Lambda_a = [a_1, \ldots, a_n]$, $\Lambda_b = [b_1, \ldots, b_n]$ and let Ω_a, Ω_b denote the unit cells spanned by the respective basis (as in Lemma 5.1, after eventual global shifts). We have $\det \{a_1, \ldots, a_n\} = \pm \det \{b_1, \ldots, b_n\}$.

We proceed by recurrence on the dimension n.

If $n = 1$, the result is obvious since Λ_a and Λ_b must be equal to have the same density. Consider now the n-dimensional case and assume the property is true up to dimension $n - 1$.

Let u be a unit vector provided by Lemma 5.1 and set $r = (\mathrm{diag}_a, u) = (\mathrm{diag}_b, u)$. Let H be the orthogonal complement of the line $\mathrm{U} = \mathbb{R} \cdot u$. The related pair of complementary projectors is given by

$$p_u(x) = (x, u)\, u\,,$$
$$p_{\mathrm{H}}(x) = x - (x, u)\, u\,.$$

Note that both unit cells project onto the same interval $[-r/2, r/2)$ in U.
Partition the space $\mathbb{R}^n$ into slices S_k, k in $\mathbb{Z}$,

$$\mathrm{S}_k = \{x \text{ in } \mathbb{R}^n \mid (k - 1/2)\, r \leq (x - t, u) < (k + 1/2)\, r\}\ ;$$

a generic shift t is put here to insure that no lattice node falls on the boundaries of those strips. For each k and $i = a, b$, $p_{\mathrm{H}}(\mathrm{S}_k \cap \Lambda_i)$ is a codimension 1 canonical tiling. By corollary 3.4 there is a lattice L_i in H and a displacement $f_{i,k}$ from the projected pattern to L_i (by including a shift in $f_{i,k}$ the lattice L_i can be chosen independent of k). Now L_a and L_b are $(n - 1)$-dim. lattices with the same density $(= r \cdot n(\Lambda_a) = r \cdot n(\Lambda_b))$. By the recurrence hypothesis there is a displacement f': $\mathrm{L}_a \leftrightarrow \mathrm{L}_b$, so that in each slice S_k a bounded one to one mapping between $\Lambda_a \cap \mathrm{S}_k$ and $\Lambda_b \cap \mathrm{S}_k$ can be constructed. So an overall displacement f is obtained. QED

6. Conclusion.

We have shown under what circumstances quasiperiodic systems built by general section methods, that is by cut of a periodic set of arbitrary (reasonable) atomic surfaces or by the

related cut and project algorithm, can be mapped in a displacive way onto a periodic pattern.

By periodicity in the higher dimensional space, the atomic surfaces may be considered modulo the n-D lattice (i.e. projected into the torus T^n). In the example of modulated crystals, these surfaces are closed manifolds without boundaries and can be deformed into a d'-dimensional torus in the torus T^n. In the case of quasicrystals, it has been argued by several authors that the atomic surfaces actually are closed manifolds in T^n [20-22]. Any closed d'-D surface can be decomposed in the way stated in theorem 4.1. So our net result is that the correspondence with a lattice exists when the atomic surface is a union of *closed* manifolds in T^n.

We conjecture that this condition, which we have proved to be sufficient, is also necessary. This is indeed the case in one dimension as a corollary of Kesten's theorem.

Another interest in the average lattice is that it provides a local, and numerically efficient, algorithm to build the quasiperiodic pattern [23]. If we know both the reference lattice and the displacements as a function of the lattice node — as in the instances where it is a modulation — then it is straightforward to recover the quasiperiodic structure.

One might also think of using the map to a lattice to treat some statistical mechanical problems on quasi-lattices. At least to the extend where the physical properties do not depend so much on the detailed topology of the network as on the range of the interactions, we may expect to get insight to solutions through such mappings.

Appendix.

An example : the mean lattice of the octagonal tiling.

The octagonal tiling is obtained by the cut and project method from $\mathbb{R}^4$ in which we consider the hypercubic lattice $\Lambda = \mathbb{Z}^4$ with the standard orthonormal basis $\{a_1, \ldots, a_4\}$. The two orthogonal planes E and E′ are defined as the ranges of the following orthogonal projectors :

$$p = \frac{1}{2}\begin{pmatrix} 1 & 0 & \alpha & -\alpha \\ 0 & 1 & \alpha & \alpha \\ \alpha & \alpha & 1 & 0 \\ -\alpha & \alpha & 0 & 1 \end{pmatrix} \quad \text{and} \quad p' = \frac{1}{2}\begin{pmatrix} 1 & 0 & -\alpha & \alpha \\ 0 & 1 & -\alpha & -\alpha \\ -\alpha & -\alpha & 1 & 0 \\ \alpha & -\alpha & 0 & 1 \end{pmatrix}$$

where $\alpha = 1/\sqrt{2}$.

The projections $L = p(\Lambda)$ and $L' = p'(\Lambda)$ are dense $\mathbb{Z}$-modules respectively generated by $\{e_1, \ldots, e_4\}$ and $\{e'_1, \ldots, e'_4\}$ where $e_i = p(a_i)$ and $e'_i = p'(a_i)$. In orthonormal coordinates

$$\begin{aligned} e_1 &= \alpha \cdot (1, 0) & e'_1 &= \alpha \cdot (1, 0) \\ e_2 &= \alpha \cdot (0, 1) & e'_2 &= \alpha \cdot (0, 1) \\ e_3 &= \alpha \cdot (\alpha, \alpha) = (1/2, 1/2) & e'_3 &= \alpha \cdot (-\alpha, -\alpha) = (-1/2, -1/2) \\ e_4 &= \alpha \cdot (-\alpha, \alpha) = (-1/2, 1/2) & e'_4 &= \alpha \cdot (\alpha, -\alpha) = (1/2, -1/2) . \end{aligned}$$

The octagonal tilings correspond to a strip $S = E \times W$ where W is the octagon obtained as the projection $p'(\Omega)$ of the unit cube of $\mathbb{R}^4$. W is the zonohedra generated by the four vectors $\{e'_1, \ldots, e'_4\}$ (see Fig. 3).

W is not a fundamental domain for any tiling of E′ and consequently, the construction given in theorem 3.1 cannot apply directly. However the octagon can be cut in two pieces, an hexagon W_H and a « boat » W_B, shown in figure 3, which are prototiles. More precisely, W_H is a unit cell for the 2-dimensional lattice L'_H generated by $h'_1 = e'_1 - e'_3$ and $h'_2 = e'_3 + e'_4$ whereas W_B is a unit cell for the 2-dimensional lattice L'_B generated by $b'_1 = e'_1 - e'_3 + e'_4$ and $b'_2 = e'_2$.

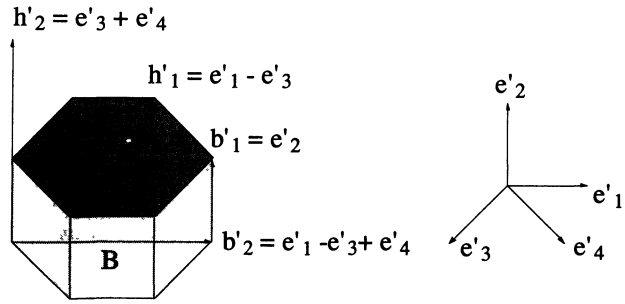

Fig. 3. — The projection of the unit cube of $\mathbb{R}^4$ is a regular octagon which can be decomposed into two pieces B and H ; B is a unit cell for the lattice generated by $\{b'_1, b'_2\}$ and H is a unit cell for $[h'_1, h'_2]$. The projected basis $\{e'_1, e'_2, e'_3, e'_4\}$ of $\mathbb{Z}^4$ is shown on the right.

Thus, if τ is a generic translation, the vertices $X_\tau = p(\Lambda_\tau \cap S)$ of the corresponding octagonal tiling can be split in two complementary subsets $X_{H,\tau}$ and $X_{B,\tau}$ respectively associated to the substrips S_H and S_B defined by $S_H = E \times W_H$ and $S_B = E \times W_B$:

$$\begin{aligned} X_{H,\tau} &= p(\Lambda_\tau \cap S_H) \\ X_{B,\tau} &= p(\Lambda_\tau \cap S_B) \\ X_\tau &= X_{H,\tau} \cup X_{B,\tau} . \end{aligned}$$

Since W_H tiles E', the general method can be applied to build a mean lattice for the structure $X_{H,\tau}$: define Λ_H as the 2-dimensional sublattice of Λ generated by $\eta_1 = a_1 - a_3$ and $\eta_2 = a_3 + a_4$ (in such a way that $L'_H = p'(\Lambda_H)$) and let E_H be the 2-dimensional lattice plane containing Λ_H.

Notice that $\{\eta_1, \eta_2, a_1, a_2\}$ is a basis of Λ and consequently $\{a_1, a_2\}$ generates a 2-dimensional sublattice which is a complement of Λ_H.

If π_H denotes the oblique projector with range E and kernel E_H then the mean lattice L_H of $X_{H,\tau}$ is the oblique projection $\pi_H(\Lambda)$ into E. Elementary linear algebra shows that L_H is generated by

$$\begin{aligned} h_1 &= \pi_H(a_1) = (2(\sqrt{2} - 1), 0) \\ h_2 &= \pi_H(a_2) = (0, 2) . \end{aligned}$$

This lattice is rectangular and the one to one mapping between $X_{H,\tau}$ and L_H is shown in figure 4a.

Similarly, define Λ_B as the 2-dimensional sublattice of Λ generated by $\beta_1 = a_1 - a_3 + a_4$ and $\beta_2 = a_2$ (so that $L'_B = p'(\Lambda_B)$) and let E_B be the 2-dimensional plane containing Λ_B.

Notice that $\{\beta_1, \beta_2, a_3, a_4\}$ is a basis of Λ.

Define π_B as the projector with range E and kernel E_B. The mean lattice L_B of $X_{B,\tau}$ is the oblique projection $\pi_B(\Lambda)$ to E and is generated by

$$\begin{aligned} b_1 &= \pi_B(a_3) = (2 - \sqrt{2}, 1) \\ b_2 &= \pi_B(a_4) = (4 - 2\sqrt{2}, 0) . \end{aligned}$$

The one to one mapping between $X_{B,\tau}$ and L_B is shown in figure 4b.

Finally the octagonal tiling X_τ can be viewed as the union of two modulated structures $X_{H,\tau}$ and $X_{B,\tau}$, each one being associated to a mean lattice. However these two lattices

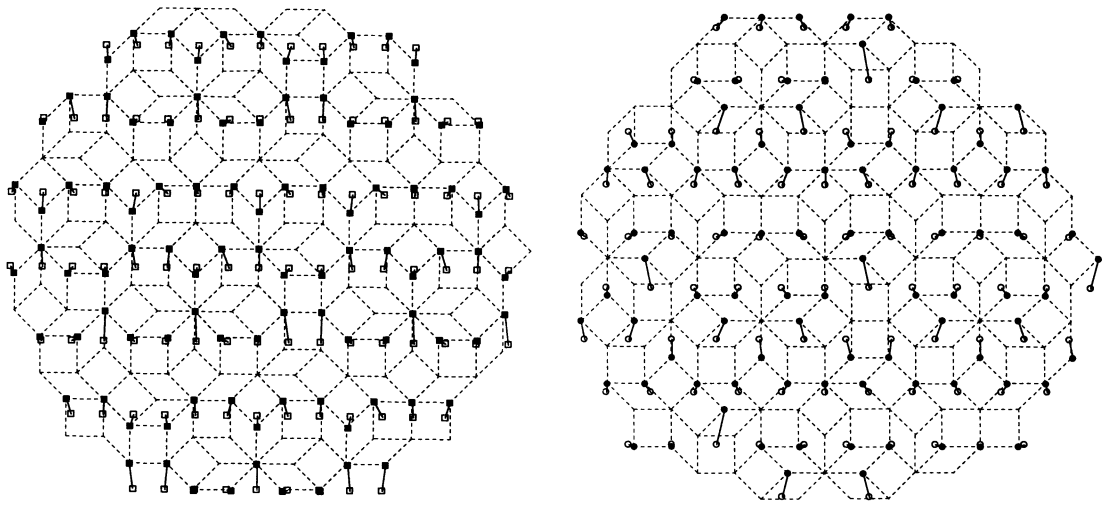

Fig. 4. — a) Black squares represent the H-part of the vertices of the octagonal tiling ; the white squares correspond to their reference lattice. b) The B-part of the tiling is represented by black dots and the corresponding reference lattice by white dots.

L_H and L_B are different and incommensurate.

The claim that the whole structure admits a unique mean lattice follows from Lemma 4.3. The final mean lattice shown in figure 5 is the centered rectangular lattice $L_H \cup [L_H + (h_1 + h_2)/2]$.

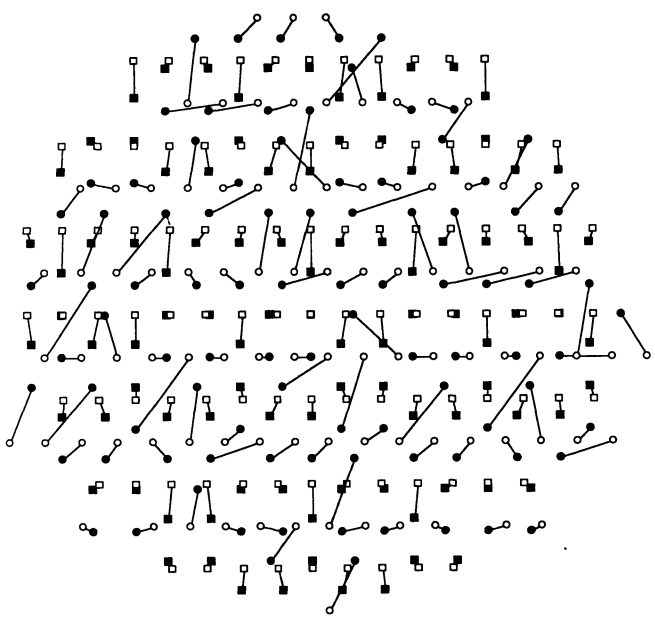

Fig. 5. — The one-to-one mapping between the octagonal tiling (black) and the rectangular centered lattice $L_H \cup [L_H + (h_1 + h_2)/2]$ (white).

A deterministic algorithm can be used to construct the octagonal tiling by means of the method explained in the previous section. We give below the main line of the construction for the $X_{H,\tau}$ structure (the $X_{B,\tau}$ structure is obtained in a similar way).

The main loop of the algorithm consists in scanning a finite subset of the square lattice of E' generated by $\{e'_1, e'_2\}$ (which is isomorphic to the mean lattice L_H).

For each $x'_1 = p_1 e'_1 + p_2 e'_2$ find the translation $y' = q_1 h'_1 + q_2 h'_2$ of the lattice L'_H such that $x' = x'_1 + y'$ belongs to the hexagonal unit cell W_H (possibly translated by a fixed translation t'). This step is the generalization of the modulo operation used in one-dimensional algorithms such as the mapping of the circle.

Then

$$x' = p_1 e'_1 + p_2 e'_2 + q_1 h'_1 + q_1 h'_1 = (p_1 + q_1) e'_1 + p_2 e'_2 + (q_2 - q_1) e'_3 + (q_1 + q_2) e'_4 ;$$

The corresponding point of the structure is readily given by

$$x = (p_1 + q_1) e_1 + p_2 e_2 + (q_2 - q_1) e_3 + (q_1 + q_2) e_4 .$$

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