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## A classification of the periodic directions in the rational approximants of icosahedral quasicrystals

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**Résumé.** — Cet article montre qu'il y a trois types de directions périodiques dans les approximants rationnels des quasicristaux icosaédriques : les directions périodiques faibles, planaires et fortes. Les critères de classification tiennent compte des propriétés de périodicité de ces directions dans l'espace direct et réciproque et aussi de l'existence de plans et de rangées atomiques, respectivement orthogonaux et parallèles à ces directions. L'ensemble de directions périodiques de tous les approximants rationnels possibles est inclus dans l'ensemble des directions du module icosaédrique qui est le réseau « Bravais » du quasicristal. Les directions de ce module sont divisées en classes de compatibilité, qui peuvent être indexées par la série de nombres libres de carrés et de la forme  $5x^2 - y^2$ ,  $x, y \in \mathbb{Z}$ .

**Abstract.** — This paper shows that there are three types of periodic directions in the rational approximants of an icosahedral quasicrystal : weakly, planar and strongly periodic directions. The classifying criteria take into account the periodicity properties of these directions in the direct and the reciprocal space, as well as the existence of atomic planes and atomic rows, orthogonal, respectively parallel to these directions. The set of periodic directions of all the possible rational approximants are module directions in the icosahedral  $\mathbb{Z}$ -module which is the « Bravais » lattice of the icosahedral quasicrystal. These module directions belong to some compatibility classes, which are indexed by the series of square-free numbers of the form  $5x^2 - y^2$ ,  $x, y \in \mathbb{Z}$ .

### 1. Introduction.

The efforts made to discover new alloy systems which exhibit long-range quasicrystalline order and non-crystallographic symmetry in certain domains of concentration and temperature showed that the quasicrystalline phase competes with the so-called rational approximant phases that are built locally with the same type of atomic clusters as the quasicrystals, but have periodic long-range order and crystallographic symmetry (see for instance Ref. [1]).

The intimate structural relationship between approximants and quasicrystals has as a consequence the fact that the quasicrystalline grains develop easily on the approximant phase grains by peritectic reactions, keeping a strong orientation relationship with the approximant

phase [2]. A whole set of intermediate phases, changing from quasicrystal to the approximant was observed at the interface between the two limiting phases [3]. Unusual shear plane orientations, which are connected more to the quasicrystalline lattice than to the crystalline approximant, Bravais lattice seem to be preferred by the stacking fault networks which were observed in the approximants [4].

The natural framework for studying the above properties is the cut and projection method, which uses the same 6-D crystal in order to describe the quasicrystal and its rational approximants (see Refs. [5, 6] for this method).

The cut and projection method is used here in order to classify the set of periodic directions in the direct and the reciprocal space of the rational approximants of an icosahedral quasicrystal. What lies behind this classification of periodic directions is the statement (valid not only for rational approximants of quasicrystals, but for all crystals in general) that a periodic direction in the direct space is not always a periodic direction in the reciprocal space and reciprocally, a periodic direction in the reciprocal space, i.e. the normal to a stack of atomic planes in the direct space, whose density varies periodically, is not always a periodic direction in the direct space. Other classifications of rational directions in approximants, discussing symmetry properties, can be found in reference [7].

As shown in references [8, 9] atomic planes and rows are present in the quasicrystal. Some of these atomic planes and rows exist also in the rational approximants, and are parallel to related planes and rows in the quasicrystal. This fact is essential for the relationship between quasicrystals and approximants and it is used as a starting point in the discussion.

This paper continues and develops ideas first presented in reference [10] and has the following structure : section 2 defines the necessary geometrical objects, following the lines of references [5] and [6]. Section 3 contains the classification of the periodic directions in the rational approximants. In section 4 the possibility of simultaneous strong periodic directions is discussed and the set of periodic directions in the rational approximants is described. A classification of the module directions in the « Bravais lattice » of the icosahedral quasicrystal is proposed, based on some arithmetic properties of this module. Section 5 discusses reflexion conditions for the diffraction patterns of rational approximants. Section 6 uses the example of a rhombohedral approximant as an illustration of the concepts developed in this paper.

## 2. Definitions and settings.

The 6-D hyperspace  $\mathbb{R}^6$ , which contains the 6-D lattice  $\mathcal{L}$ , is decomposed into two 3-D hyperplanes  $P^{\parallel}$ ,  $P^{\perp}$ , invariant with respect to the action of the icosahedral group [5] :  $\mathbb{R}^6 = P^{\parallel} \oplus P^{\perp}$  ;  $P^{\parallel}$  is the *physical or the tiling space*, which contains the projected structure,  $P^{\perp}$  is the *orthogonal or the internal space*, which contains the acceptance domain, i.e. the cross section of the strip, for a perfect icosahedral quasicrystalline structure.  $\mathcal{L}$  may be a P, F, or I hypercubic lattice, as shown in [11].  $\mathbb{R}^6$  may also be considered as reciprocal space and contains the reciprocal lattice  $\mathcal{L}^*$  which is respectively a P, I, or F hypercubic lattice. Different structures, quasicrystalline and crystalline, can be obtained by tilting the strip and introducing two new 3-D hyperplanes  $P^a$ ,  $P^g$  ( $\mathbb{R}^6 = P^g \oplus P^a$ ) ;  $P^g$  is the *grid space* [6], parallel to the strip and  $P^a$  is the *acceptance space*, transversal to the strip, which contains the acceptance domain of the inclined strip structures. The quasicrystalline icosahedral structure is obtained with a nontilted strip, parallel to  $P^{\parallel}$ . Rational approximant structures correspond to special values of the slopes of the grid space  $P^g$  [6, 15, 16].

The 6-D hypercubic lattice  $\mathcal{L}$  projects orthogonally onto  $P^{\parallel}$  and  $P^{\perp}$  and gives two dense modules,  $\mathcal{L}^{\parallel}$  and  $\mathcal{L}^{\perp}$  respectively which have icosahedral symmetry (see [5]).  $\mathcal{L}^{\parallel}$  is the « *Bravais lattice* » of the icosahedral quasicrystalline tiling, i.e. the set of all its quasiperiods. Both the modules  $\mathcal{L}^{\parallel}$  and  $\mathcal{L}^{\perp}$  are isomorphic with  $\mathcal{L}$  and mutually isomorphic. The natural isomorphism

$\tilde{\delta}$  (defined in Refs. [5, 8, 9] as  $\tilde{\delta} = \Pi^\perp (\Pi^\parallel)^{-1}$ , where  $\Pi^\parallel$ ,  $\Pi^\perp$  are orthogonal projectors onto  $\mathcal{P}^\parallel$ ,  $\mathcal{P}^\perp$ ) between  $\mathcal{L}^\parallel$  and  $\mathcal{L}^\perp$  is nowhere continuous and therefore cannot be extended to an affine transformation from  $\mathcal{P}^\parallel$  to  $\mathcal{P}^\perp$ ; it has nevertheless the property that it transforms module directions and planes of  $\mathcal{L}^\parallel$  into module directions and planes of  $\mathcal{L}^\perp$  [5, 8, 9]. The module directions and planes generalize the lattice directions and planes from classical crystallography, as cuts of affine dimension 1, respectively 2 in the Bravais lattice. The difference between the classical crystallographic concepts and their quasicrystallographic correspondents consists in the fact that a module direction in an icosahedral module have rank (module dimension) 2, being the projection on the physical space of a 2-D hyperlattice plane, and that the module planes in an icosahedral module have rank 4, being the projection onto the physical space of a 4-D hyperlattice plane (see Refs. [5, 8, 9]).

Projecting  $\mathcal{L}$  onto  $\mathcal{P}^a$  we obtain a new module  $\mathcal{L}^a$  which has rank 3, being no longer dense, in the case of a rational approximant. In this case,  $\tilde{\gamma}^a = \Pi^a (\Pi^\parallel)^{-1}$  ( $\Pi^a$  is the orthogonal projector on  $\mathcal{P}^a$ ) defines only a homomorphism from  $\mathcal{L}^\parallel$ , onto  $\mathcal{L}^a$ . Finally, projecting  $\mathcal{L}^*$  obliquely onto  $\mathcal{P}^\parallel$  along  $\mathcal{P}^a$ , and orthogonally on  $\mathcal{P}^\parallel$  we obtain the modules  $\mathcal{L}^d$ ,  $\mathcal{L}^{\parallel*}$ , respectively, which are the Fourier modules of the inclined strip structure and of the icosahedral structure, respectively [12]. The natural homomorphism  $\tilde{\gamma}^d = \Pi^d (\Pi^\parallel)^{-1}$  from  $\mathcal{L}^{\parallel*}$  onto  $\mathcal{L}^d$  describes what are usually called « diffraction peak shifts » [12].

The following definitions concern 2-planes in the 6-D hyperspace which are connected, to module directions in  $\mathcal{L}^\parallel$  and in  $\mathcal{L}^\perp$ , as shown in references [5, 8, 9].

A 2-plane in the 6-D hyperspace is called a « transversal plane » (TP) if it intersects  $\mathcal{P}^\parallel$  along a direction  $\mathbf{d}^\parallel$  and  $\mathcal{P}^\perp$  along a direction  $\mathbf{d}^\perp$ . A TP which is also a hyperlattice 2-plane (i.e. a 2-D lattice plane of  $\mathcal{L}$ ) is called a « hyperlattice transversal plane » (HTP).

*Theorem 1.* — A TP is a HTP if  $\mathbf{d}^\parallel$  and  $\mathbf{d}^\perp$  are the projections of the same hyperlattice direction  $\mathbf{d}$  (i.e. lattice direction of  $\mathcal{L}$ ) on  $\mathcal{P}^\parallel$  and  $\mathcal{P}^\perp$ , respectively. In this case  $\mathbf{d}^\parallel$ ,  $\mathbf{d}^\perp$  are module directions in the modules  $\mathcal{L}^\parallel$ ,  $\mathcal{L}^\perp$ . The module directions  $\mathbf{d}^\parallel$  and  $\mathbf{d}^\perp$  are the supports of the projections onto  $\mathcal{P}^\parallel$  and  $\mathcal{P}^\perp$ , respectively of all the points of the 2-D HTP in  $\mathcal{L}$  and because of their irrational inclination in this HTP, they have rank 2 (the positions of the projected points are linear combinations with integer coefficients of two incommensurate lengths). Given a module direction  $\mathbf{d}^\parallel$  in  $\mathcal{L}^\parallel$  there is always a unique module direction  $\mathbf{d}^\perp$  in  $\mathcal{L}^\perp$  such that the plane formed by  $\mathbf{d}^\parallel$  and  $\mathbf{d}^\perp$  is a HTP. Equivalently, for a given hyperlattice direction  $\mathbf{d}$  there is one and only one HTP which passes through this direction (for the proof see [5]).

### 3. Strongly, weakly and planar periodic directions.

The definitions of TP's and HTP's do not depend on the strip and pertain in fact only to the modules  $\mathcal{L}^\parallel$ ,  $\mathcal{L}^\perp$ . Nevertheless, the vertices of the projected structure form a discrete subset of points of  $\mathcal{L}^\parallel$ , whose selection depends on the inclination of the strip, and some set of module directions  $\mathbf{d}^\parallel$  could be differentiated in a way specified by the theorems 2 and 3 (the proofs of which can be found in appendix A).

*Theorem 2.* — The following statements are equivalent :

- i) the intersection of the HTP corresponding to  $\mathbf{d}^\parallel$  with the grid space  $\mathcal{P}^g$  is a direction  $\mathbf{d}^g$ ;
- ii) the homomorphism  $\tilde{\gamma}^d$  from  $\mathcal{L}^{\parallel*}$  onto  $\mathcal{L}^d$  transforms the module planes orthogonal to  $\mathbf{d}^\parallel$  in  $\mathcal{L}^{\parallel*}$  onto module planes orthogonal to  $\mathbf{d}^\parallel$  in  $\mathcal{L}^d$ . Particularly, the module plane orthogonal to  $\mathbf{d}^\parallel$ , which passes through the origin of the reciprocal space is conserved by this homomorphism ;

iii) all the module directions parallel to  $\mathbf{d}^l$  in  $\mathcal{L}^l$  are transformed onto directions parallel to the same vector in  $\mathcal{L}^a$  by the natural homomorphism  $\mathcal{F}^a$ .

*Discussion :*

i) the situation in which the intersection between the HTP and  $P^g$  is a line is rather special, because the intersection between a 3-D plane and a 2-D plane can be a point, a line, or a 2-D plane ; for any inclination of the 3-D plane  $P^g$  there is an infinitesimal variation of its slopes which makes the above intersection a point. Another remark is that a direction  $\mathbf{d}^g$  belonging to  $\mathcal{L}$ , implies direct space periodicity along  $\mathbf{d}^l$  ;

ii) states that the diffraction peak shifts conserve the plane which passes through the origin of the reciprocal space and is orthogonal to a direct space periodicity direction. We have identified here the set of directions of  $\mathcal{L}^{l*}$  with the set of directions of  $\mathcal{L}^l$  (this fact is not trivial, as can be seen later for 3-D periodic lattices, and is due to the high symmetry of the lattice  $\mathcal{L}$ ) ;

iii) is intimately connected to the existence of rows and channels in the projected structure. To see this the following definition and lemma is needed.

An acceptance space  $P^a$  has the *finite extension - discrete distribution* (FE-DD) property if all the subsets of  $\mathcal{L}$  which project orthogonally onto bounded sets of the acceptance space have orthogonal projections on the physical space which are discretely distributed.

Lemma 1 :  $P^a$  has the FE-DD property if  $P^g \cap P^\perp = \{0\}$ .

For the proof of this lemma, let us first consider a bounded volume  $\mathcal{V}^l$  in the physical space. The vertices of  $\mathcal{L}$  which are orthogonally projected onto this volume, and whose orthogonal projections onto  $P^a$  belong to a bounded set  $\mathcal{V}^a$ , come from a set  $\mathcal{V}$  which is the intersection of two cylinders : one with basis  $\mathcal{V}^l$  and generated by  $P^\perp$ , the other one with basis  $\mathcal{V}^a$  and generated by  $P^g$ . The set  $\mathcal{V}$  is bounded and therefore contains a finite number of hyperlattice vertices if the generators of the two cylinders have no common directions.

The module  $\mathcal{L}^l$  which is the support of the projected structure contains a dense set of directions parallel to a given module direction  $\mathbf{d}^l$ . If  $\mathbf{d}^l$  satisfies the condition iii) of theorem 2 then these directions are carried by the homomorphism  $\mathcal{F}^a$  onto a bundle of parallel lines in the acceptance space  $P^a$ . The part of this bundle of lines in  $P^a$ , which cuts the acceptance domain, is bounded in the dimension transversal to the bundle (of course, for a bounded acceptance domain). If  $P^a$  has the FE-DD property then the lines in  $\mathcal{L}^l$  which are not empty, have a discrete distribution in  $P^a$ . Therefore, in the case of a bounded acceptance domain and of an acceptance space with the FE-DD property, if we look along a direct space periodicity direction we can see rows and channels.

*Theorem 3.* — The following statements are equivalent :

i) the intersection of the HTP corresponding to  $\mathbf{d}^l$  with the acceptance space  $P^a$  is a direction  $\mathbf{d}^a$  ;

ii) the homomorphism  $\mathcal{F}^d$  from  $\mathcal{L}^l$  onto  $\mathcal{L}^d$  transforms all module directions parallel to  $\mathbf{d}^l$  onto module directions parallel to  $\mathbf{d}^d$ . Particularly, the module direction  $\mathbf{d}^l$  which passes through the origin is conserved ;

iii) all the module planes, orthogonal to  $\mathbf{d}^l$  in  $\mathcal{L}^l$  are transformed into planes orthogonal to a given vector in  $\mathcal{L}^a$  by the homomorphism  $\mathcal{F}^a$ .

*Discussion :*

i) the same remark on the dimension of the intersection as that for statement 2 i) is valid. Also, if  $\mathbf{d}^a$ , which is a direction of oblique projection parallel to  $P^a$ , belongs to  $\mathcal{L}$ , then the Fourier module  $\mathcal{L}^d$ , obtained by this projection, is periodic along  $\mathbf{d}^l$  ;

ii) states that the diffraction peaks shifts preserve reciprocal space periodic directions ;  
 iii) states that for a module direction which satisfies the conditions of theorem 3, the vertices of the projected structure are distributed on planes, stacked orthogonally to  $\mathbf{d}^{\parallel}$ , and have a discrete distribution along  $\mathbf{d}^{\parallel}$ , provided that the acceptance domain is bounded and that the FE-DD condition is fulfilled.

Suppose in the following that the FE-DD property is valid ; this occurs in all normal cases, i.e. when  $P^{\mathcal{E}}$  has an inclination not very different from  $P^{\parallel}$ .

A module direction  $\mathbf{d}^{\parallel}$  which satisfies the conditions of the theorem 2, i.e. there is a direction  $\mathbf{d}^{\mathcal{E}}$  belonging to the grid space and also to the HTP corresponding to  $\mathbf{d}^{\parallel}$  with  $\mathbf{d}^{\mathcal{E}}$  a hyperlattice direction, but does not satisfy the conditions of the theorem 3, i.e. there is no direction  $\mathbf{d}^{\mathcal{A}}$ , is called *weakly periodic* ; the tiling is in this case periodic along  $\mathbf{d}^{\parallel}$  in the direct space, but the projection on  $\mathbf{d}^{\parallel}$  of all the vertices in the tiling is dense ; nevertheless, the projection of all the vertices of the tiling on the plane orthogonal to this direction is discrete and we can see channels if we look along  $\mathbf{d}^{\parallel}$ . A module direction  $\mathbf{d}^{\parallel}$  which satisfies the conditions of theorem 3 (i.e. there is a direction  $\mathbf{d}^{\mathcal{A}}$  belonging to the grid space and also to the HTP corresponding to  $\mathbf{d}^{\parallel}$ , with  $\mathbf{d}^{\mathcal{A}}$  a hyperlattice direction) but does not satisfy the conditions of theorem 2 (i.e. there is no direction  $\mathbf{d}^{\mathcal{E}}$ ) is called *planar periodic* ; the vertices of the tiling are distributed on non-equivalent planes, orthogonal to  $\mathbf{d}^{\parallel}$ , whose density varies periodically along  $\mathbf{d}^{\parallel}$ , which is a *periodic direction in the reciprocal space*. In this case we no longer have channels along  $\mathbf{d}^{\parallel}$ . Finally, a module direction  $\mathbf{d}^{\parallel}$  which satisfies the conditions of both theorems 2 and 3 (i.e. the grid space and the acceptance space both intersect the HTP corresponding to  $\mathbf{d}^{\parallel}$  along hyperlattice directions  $\mathbf{d}^{\mathcal{E}}$  and  $\mathbf{d}^{\mathcal{A}}$ ) is called *strongly periodic* ; in this case planes stack along  $\mathbf{d}^{\parallel}$  and the period of the density of such planes is a submultiple of the period of the tiling along  $\mathbf{d}^{\parallel}$ , which is a *periodic direction both in direct and reciprocal space* ; channels along  $\mathbf{d}^{\parallel}$  can also be seen.

#### 4. Simultaneous strongly periodic directions.

In the quasicrystalline icosahedral structure, all module directions are « strong », in the sense that they satisfy the conditions of both theorems 2 and 3 (in this case  $P^{\mathcal{E}} = P^{\parallel}$  and  $P^{\mathcal{A}} = P^{\perp}$ ,  $\mathbf{d}^{\mathcal{E}} = \mathbf{d}^{\parallel}$  and  $\mathbf{d}^{\mathcal{A}} = \mathbf{d}^{\perp}$ ) although they are neither weakly periodic, nor planar periodic. To induce periodicity we must tilt the strip and automatically lose the strong character of a part of the above module directions. As the HTP corresponding to a strongly periodic direction  $\mathbf{d}^{\parallel}$  must have a direction  $\mathbf{d}^{\mathcal{E}}$  in  $P^{\mathcal{E}}$  and a direction  $\mathbf{d}^{\mathcal{A}}$  in  $P^{\mathcal{A}}$ , the rotation which tilts the strip must keep this HTP globally invariant, passing from  $\mathbf{d}^{\parallel}$  to  $\mathbf{d}^{\mathcal{E}}$  and from  $\mathbf{d}^{\perp}$  to  $\mathbf{d}^{\mathcal{A}}$ , in order to preserve the strong character of  $\mathbf{d}^{\parallel}$ . Rotations in 6-D always have three mutually orthogonal, invariant 2-planes [13]. We can choose these three 2-planes as HTP,  $\mathcal{K}_i$ ,  $i = 1, 3$  corresponding to three mutually orthogonal strongly periodic directions  $\mathbf{d}^{\parallel}_i$ ,  $i = 1, 3$  ; in each of these HTP we choose rotation angles equal to the angle between  $\mathbf{d}^{\parallel}_i$ ,  $i = 1, 3$ , and the hyperlattice directions  $\mathbf{d}^{\mathcal{E}}_i$  in  $\mathcal{K}_i$ ,  $i = 1, 3$ . The resulting structure is a rational approximant, which contains at least three strongly periodic directions.

*Theorem 4.* — A necessary condition to have more than three strongly periodic directions is that the rotation angles in at least two mutually orthogonal invariant HTP should be equal in absolute values (the angle condition). In this case the rotation which tilts the strip has a continuous set of invariant 2-planes, and a countable subset of this set of invariant 2-planes are HTP corresponding to strongly periodic directions. When the absolute values of the rotation angles are equal in all three HTP, then the additional strongly periodic directions are distributed in the entire physical space, otherwise they are restricted to that 2-plane in the physical space which contains the two module directions which satisfy the angle condition (for the proof see [13]).

**4.1 THE ANGLE CONDITION AND THE COMPATIBILITY CLASSES OF MODULE DIRECTIONS.** — This subsection shows that the angle condition cannot be fulfilled by any pair of module directions in  $\mathfrak{L}^{\parallel}$ . First of all, let us consider the distribution of the slopes of the hyperlattice directions in different HTP's.

Starting with some primitive hyperlattice direction,  $\mathbf{d} \in \mathfrak{L}$ , all the other hyperlattice directions in the same HTP,  $\mathfrak{H}(\mathbf{d})$  as  $\mathbf{d}$ , can be generated by applying to  $\mathbf{d}$  all the elements of the group of the matrices with integer coefficients which leave all HTP's invariant (see also Ref. [14])

$$T_{p,q} = p + q \sqrt{5}(\Pi^{\parallel} - \Pi^{\perp}), \quad p, q \in \mathbb{Z}. \quad (1)$$

The period  $P(p, q; \mathbf{d})$  along  $\mathbf{d}^{\parallel}$  depends on the hyperlattice vector  $\mathbf{d}_{p,q} = T_{p,q} \mathbf{d}$  in  $\mathfrak{H}(\mathbf{d})$ , with which the strip was chosen to be parallel, and is equal to the projection of  $\mathbf{d}_{p,q}$  on  $\mathbb{P}^{\parallel}$ , divided by some integer factor  $k(p, q; \mathbf{d})$ . The presence of this factor comes from the fact that the 2-D lattice  $\mathfrak{L}(\mathbf{d})$  generated by  $\mathbf{d}$  and  $\sqrt{5}(\Pi^{\parallel} - \Pi^{\perp}) \mathbf{d}$  might have an index  $i(\mathbf{d})$  different from 1 in the 2-D lattice  $\mathfrak{L} \cap \mathfrak{H}(\mathbf{d})$ , and the vector  $\mathbf{d}_{p,q}$  might be nonprimitive. Of course,  $k(p, q; \mathbf{d})$  is some factor of  $i(\mathbf{d})$ , depending on  $\mathfrak{L}$  being a P, F, or I lattice, and can be found by solving a system of Diophantine equations (see Refs. [15, 16])

$$P(p, q; \mathbf{d}) = \frac{(q \sqrt{5} + p)}{k(p, q; \mathbf{d})} P(\mathbf{d}) \quad (2)$$

where  $P(\mathbf{d}) = ((x(\mathbf{d}) \sqrt{5} + y(\mathbf{d}))/2 \sqrt{5})^{1/2}$  and  $\mathbf{d}$  is considered to be primitive ;

$$x(\mathbf{d}) = |\mathbf{d}|^2 \quad \text{and} \quad y(\mathbf{d}) = \sqrt{5}(|\Pi^{\parallel} \mathbf{d}|^2 - |\Pi^{\perp} \mathbf{d}|^2)$$

are integers if the edge length of the 6-D hypercube is equal to 1 for a P lattice or to 2 for an F or an I lattice.

The slope of  $\mathbf{d}_{p,q}$  with respect to  $\mathbf{d}^{\parallel}$ ,  $\text{tg } \theta(p, q; \mathbf{d})$  is equal, up to a sign, to  $|\Pi^{\parallel} \mathbf{d}_{p,q}| / |\Pi^{\perp} \mathbf{d}_{p,q}|$  :

$$\text{tg } \theta(p, q; \mathbf{d}) = \frac{(p - q \sqrt{5})}{(p + q \sqrt{5})} \text{tg } \theta(\mathbf{d}) \quad (3)$$

where  $\text{tg } \theta(\mathbf{d})$  is the slope of  $\mathbf{d}$  with respect to  $\mathbf{d}^{\parallel}$  ;  $\text{tg } \theta(\mathbf{d}) = ((\sqrt{5} x(\mathbf{d}) - y(\mathbf{d})) / (\sqrt{5} x(\mathbf{d}) + y(\mathbf{d})))^{1/2}$  (see [17]).

Two module directions  $\mathbf{d}_i^{\parallel}$ ,  $i = 1, 2$  and their corresponding HTP,  $\mathfrak{H}_i$ ,  $i = 1, 2$  are called *compatible* if the distribution (3) of slopes is the same for both module directions. A necessary and sufficient condition for compatibility is :

$$\left( \frac{\sqrt{5} x(\mathbf{d}_1) - y(\mathbf{d}_1)}{\sqrt{5} x(\mathbf{d}_1) + y(\mathbf{d}_1)} \times \frac{\sqrt{5} x(\mathbf{d}_2) + y(\mathbf{d}_2)}{\sqrt{5} x(\mathbf{d}_2) - y(\mathbf{d}_2)} \right)^{1/2} = \frac{(p - q \sqrt{5})}{(p + q \sqrt{5})} \quad \text{for any } p, q \in \mathbb{Z}. \quad (4)$$

This gives a system of equations for  $p$  and  $q$  which have integer solutions if and only if :

$$(5 x^2(\mathbf{d}_1) - y^2(\mathbf{d}_1)) / (5 x^2(\mathbf{d}_2) - y^2(\mathbf{d}_2)) = (k/\ell)^2, \quad \text{for any } k, \ell \in \mathbb{Z}. \quad (5)$$

The module directions and their corresponding HTP are divided into *compatibility classes* which are indexed by a series of *square-free numbers*  $s$  (i.e. numbers which have no square divisors) ; the HTP belonging to a class  $s$  contain hyperlattice directions  $\mathbf{d}$  such that :

$$5 x^2(\mathbf{d}) - y^2(\mathbf{d}) = s n^2(\mathbf{d}). \quad (6)$$

As shown in reference [18], not all numbers can be represented as  $5x^2 - y^2$ , with  $x, y \in \mathbb{Z}$ . The representable square free numbers  $s$  take the values 1, 5, 11, 19, 29, 31, 41, . . .

The square root of  $5x^2(\mathbf{d}) - y^2(\mathbf{d})$  has a geometrical meaning, being the surface of the unit cell of  $\mathcal{L}(\mathbf{d})$  and therefore equal to the index  $i(\mathbf{d})$  times the surface of the primitive unit cell of  $\mathcal{L} \cap \mathcal{H}(\mathbf{d})$ .

The class  $s = 1$  contains the 2-fold and the 3-fold axes of the icosahedron and the class  $s = 5$  contains the 5-fold axes of the icosahedron.

If two module directions belong to the same compatibility class, the angle condition can be fulfilled for all the values (3) of the slopes (which form an infinite countable set). If the module directions belong to different compatibility classes, the angle condition cannot be satisfied for any of the values (3) of the slopes.

**4.2 THE SETS OF PERIODIC DIRECTIONS.** — Coming back to theorem 4, let us show that the angle condition is also sufficient for the existence of more than three strongly periodic directions in a rational approximant. Consider again the three module directions  $\mathbf{d}_i^{\parallel}$ ,  $i = 1, 3$  and strong periodicity with periods  $P(\mathbf{d}_i)$ ,  $i = 1, 3$ , on all these three directions.

The direct space periodicity directions form a set  $D$  :

$$D = \{z_1 P(\mathbf{d}_1) : z_2 P(\mathbf{d}_2) : z_3 P(\mathbf{d}_3) \mid z_i \in \mathbb{Z}, i = 1, 3 \} . \tag{7}$$

The set of reciprocal space periodicity directions is :

$$D^* = \{z_1/P(\mathbf{d}_1) : z_2/P(\mathbf{d}_2) : z_3/P(\mathbf{d}_3) \mid z_i \in \mathbb{Z}, i = 1, 3 \} . \tag{8}$$

The strongly periodic directions form the set  $D^s$  :

$$D^s = D \cap D^* \tag{9}$$

The set of weakly periodic directions is  $D - D^s$  and the set of planar periodic is  $D^* - D^s$ . Note that  $D$ ,  $D^*$  and  $D^s$  do not change when the ratios  $P(\mathbf{d}_1) : P(\mathbf{d}_2) : P(\mathbf{d}_3)$  are multiplied by rational factors.

Suppose that at least  $\mathbf{d}_1$  and  $\mathbf{d}_2$  satisfy the angle condition. This imposes some restrictions on the ratio  $P(\mathbf{d}_1)/P(\mathbf{d}_2)$  which are summarized by theorem 5 (see the proof in Appendix B).

*Theorem 5.* — If

$$\text{tg } \theta(\mathbf{d}_1) = \text{tg } \theta(\mathbf{d}_2) \tag{10a}$$

then

$$(P(\mathbf{d}_1)/P(\mathbf{d}_2))^+ = (n(\mathbf{d}_1)/n(\mathbf{d}_2))^{1/2} \tag{11}$$

where  $n(\mathbf{d}_1)$ ,  $n(\mathbf{d}_2)$  are integers defined in (6).

The coincidences in the distribution (3) of slopes for the HTP corresponding to  $\mathbf{d}_1$  and  $\mathbf{d}_2$  are in infinite number ; all coincidences are generated from the first considered coincidence by the operators  $T_{p,q}$ , the ratio of the periods changing only by rational factors :

$$(P(p, q ; \mathbf{d}_1)/P(p, q ; \mathbf{d}_2))^+ = (k(p, q ; \mathbf{d}_2)/k(p, q ; \mathbf{d}_1))(n(\mathbf{d}_1)/n(\mathbf{d}_2))^{1/2} \tag{12}$$

If

$$\text{tg } \theta(\mathbf{d}_1) = - \text{tg } \theta(\mathbf{d}_2) \tag{10b}$$

then the ratios (11), (12) are multiplied by  $\sqrt{5}$  or  $1/\sqrt{5}$ .



$k(p, q; \mathbf{d}_2)$  is a factor of  $i(\mathbf{d}_2)$  and  $k(p, q; \mathbf{d}_1)$  is a factor of  $i(\mathbf{d}_1)$ , so that the ratio  $k(p, q; \mathbf{d}_2)/k(p, q; \mathbf{d}_1)$  takes only a finite number of values, when  $p$  and  $q$  changes. There is only a finite number of period ratios compatible with the angle condition (see Fig. 1 for the occurrence of only two values of the ratio  $(P(\mathbf{d}_1)/P(\mathbf{d}_2))^+ = 1, 1/2$  case (10a) for  $\mathbf{d}_1^{\parallel}$  a 5-fold axis and  $\mathbf{d}_2^{\parallel}$  a  $[\tau, 1, 0]$  axis (in Cahn's indexing system [19]); in case (10b) there are only four values of the ratio  $(P(\mathbf{d}_1)/P(\mathbf{d}_2))^- = \sqrt{5}, 1/\sqrt{5}, \sqrt{5}/2, 1/2\sqrt{5}$ ).

1/P

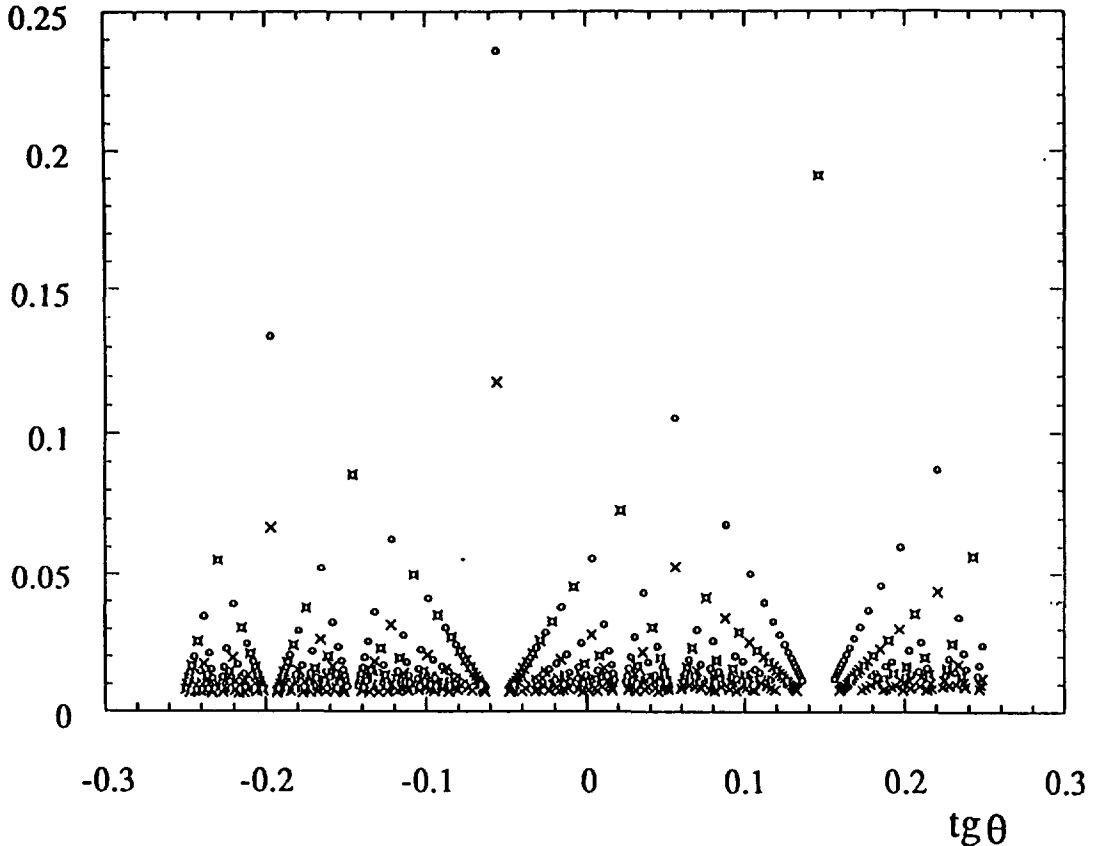


Fig. 1. — The plot of the inverse of the period  $1/P$  vs. the slope  $\text{tg } \theta$  for the hyperlattice vectors belonging to the HTP corresponding to a fivefold axis (O) and to a  $[\tau, 1, 0]$  type axis (x) in a P-type hyperlattice (the hypercube edge length is unity).

According to theorem 5, if (10a) or (10b) are fulfilled, then  $(P(\mathbf{d}_1)/P(\mathbf{d}_2))^2$  is a rational number and

$$\{z_1 P(\mathbf{d}_1) : z_2 P(\mathbf{d}_2) : 0, z_1, z_2 \in \mathbb{Z}\} = \{z_1/P(\mathbf{d}_1) : z_2/P(\mathbf{d}_2) : 0, z_1, z_2 \in \mathbb{Z}\} .$$

Using (7), (8), (9) :

$$\{z_1 P(\mathbf{d}_1) : z_2 P(\mathbf{d}_2) : 0, z_1, z_2 \in \mathbb{Z}\} \subset D^5 \tag{13}$$

which means that all the periodicity directions in the plane formed by  $\mathbf{d}_1^{\parallel}$  and  $\mathbf{d}_2^{\parallel}$  are strong.

All the period ratios compatible with relation (10a) allow the same set (13) of strongly periodic directions as they differ only by rational factors.

Nevertheless, the period ratios compatible with relation (10b) correspond to a different set of strongly periodic directions, also in the plane formed by  $\mathbf{d}_1^{\parallel}$  and  $\mathbf{d}_2^{\parallel}$ , because of the additional irrational factor  $\sqrt{5}$ .

For  $|\operatorname{tg} \theta(\mathbf{d}_1)| = |\operatorname{tg} \theta(\mathbf{d}_2)| = |\operatorname{tg} \theta(\mathbf{d}_3)|$  all the periodic directions are strong ( $D = D^* = D^s$ ).

As the transformations (1) multiply the ratios  $P(\mathbf{d}_1) : P(\mathbf{d}_2) : P(\mathbf{d}_3)$  by rational factors, they preserve the same sets of strongly, planar and weakly periodic directions. The rational approximants with the same sets of strongly, planar and weakly periodic directions form series indexed by two integers, the operators  $T_{p,q}$  acting inside the series as generalized inflation transformations. When  $p + q\sqrt{5}$  is a power of  $\tau^3$  ( $\tau = (1 + \sqrt{5})/2$  is the golden number)  $T_{p,q}$  become the usual inflation transformations which only scale the periods of the approximants, without changing their relative ratios (Refs. [20, 21]).

Although the same set of periodic directions may correspond to different space groups, there is some correlation which will not be discussed in this paper, between the set of periodic directions and the space group of the rational approximant [16].

**4.3 THE STABILITY OF THE STRONGLY PERIODIC DIRECTIONS.** — Up to now, the strong, weak, or the planar character of a module direction was associated with its periodicity, but theorems 2 and 3 are more general and also apply to quasiperiodic directions. We may say that a module direction is strong when it satisfies the conditions of both theorems 2 and 3, with no demand for the rationality of the directions  $\mathbf{d}^s$  and  $\mathbf{d}^a$  with respect to the high dimensional lattice (analogous definitions can be given for weak and planar directions). The set of all strong directions is fixed by similar angle conditions :

$$\operatorname{tg} \theta_1 = \pm \operatorname{tg} \theta_2 \quad (14a)$$

or 
$$\operatorname{tg} \theta_1 = \pm \operatorname{tg} \theta_2 = \pm \operatorname{tg} \theta_3 . \quad (14b)$$

It is possible to keep exactly the same set of strong directions, by allowing the same type of relationship as (14a) or (14b) and continuously pass, by changing the free values of the slopes ( $\operatorname{tg} \theta_1$  and  $\operatorname{tg} \theta_3$  in (14a) and  $\operatorname{tg} \theta_1$  in (14b)), through periodic and quasiperiodic structures (the periodic structures are obtained for values of the slopes of the type (3)).

This fact was discussed in connection with Schur rotations which keep a maximal symmetry subgroup [15, 22]. The most general discussion of the constraints imposed by symmetry on the slopes of the cut can be found in references [23, 24]. The number of free parameters for different symmetries of the cut (subgroups of  $Y_h$ ) is 1 for  $T_h$ , or  $D_{5d}$ , 2 for  $D_{3d}$ , 3 for  $D_{2h}$ , 5 for  $C_{2h}$  and 9 for  $S_2$ . Except for the cases  $C_{2h}$  and  $S_2$  these free parameters are rotation angles in 2-D planes corresponding to some set of strong directions which is strictly determined by the symmetry (the set of strong directions for one symmetry group includes the sets of strong directions for all its subgroups). For the cuts of lowest symmetry ( $C_{2h}$ ,  $S_2$ ) keeping at least three strong directions is a more restrictive condition than fixing the symmetry and leaves at most 3 parameters free.

## 5. Reflection conditions.

Both general (due to the Bravais lattice) and special (due to the decoration of the Bravais lattice) *reflection conditions* for the diffraction pattern of a rational approximant, are contained in the homomorphism  $\mathfrak{J}^d$  (see Appendix A Eq. (A5)). We called  $\mathfrak{L}^d$  the Fourier module and not

the reciprocal lattice because  $\mathcal{L}^d$  is the support of all non-extinct diffraction peaks (we ignore the extinctions which come from some special shape of the acceptance domain) and does not always coincide with the reciprocal lattice of the approximant which is the Fourier transform of the Bravais lattice without decoration.

Reflection conditions are defined now in a way which is non-standard, but which comes naturally in the discussion of periodic directions. Let us consider the strongly periodic direction  $\mathbf{d}^{\parallel}$ . The period in the direct space along  $\mathbf{d}^{\parallel}$  is  $P$ . The Fourier module has a period  $P^*$  along  $\mathbf{d}^{\parallel}$ . The presence of the reflection conditions implies that generically  $(PP^*)/2\pi$  is an integer  $f \neq 1$ , called *extinction factor* [10]. The effect of the Bravais lattice and of its decoration can be separated in the extinction factor

$$f = f_B f_d \tag{15}$$

where  $f_B = (PP_R^*)/2\pi$  where  $P_R^*$  is the period of the reciprocal lattice along  $\mathbf{d}^{\parallel}$ .  $P_R^*$  may eventually differ from  $P^*$

Finally note that  $P/f$  represents the period of the density of the atomic planes stacked orthogonally to  $\mathbf{d}^{\parallel}$ .

**6. The rhombohedral approximant.**

The example of a rhombohedral approximant of a  $P$  icosahedral quasicrystal (Refs. [23, 25, 26]) is now used as an illustration of the above concepts.

Three mutually orthogonal strongly periodic directions  $\mathbf{d}_i^{\parallel}$ ,  $i = 1, 3$  generate an approximant with the symmetry  $R\bar{3}m$  if the periods on  $\mathbf{d}_i^{\parallel}$ ,  $i = 1, 3$  are chosen like in table I (the indexing system for the module directions in Tab. I is chosen like in [5]). Of course, many other rhombohedral rational approximants, with different size of the unit cell, are possible [26].

Table I. — *The three mutually orthogonal strong periodic directions in a rhombohedral approximant (the hypercube edge length is unity).*

Axes	Indices	Symmetry	x	y	$5x^2 - y^2$	Period	$\mathbf{d}_g$	$\mathbf{d}_a$	$\text{tg } \theta$
$\mathbf{d}_1^{\parallel}$	[011001]	$\bar{3}$	3	6	$3^2$	$\sqrt{3}/4(3 + \sqrt{5})$ $(5 + 11/\sqrt{5})^{1/2}$	[1441 $\bar{1}$ 4]	[ $\bar{4}$ 11 $\bar{4}$ 41]	$17\sqrt{5}-38$
$\mathbf{d}_2^{\parallel}$	[000110]	2	2	2	$4^2$	$(5 + 11/\sqrt{5})^{1/2}$	[0 $\bar{1}$ 0221]	[02011 $\bar{2}$ ]	$(-11 + 5\sqrt{5})/2$
$\mathbf{d}_3^{\parallel}$	[200 $\bar{1}$ 10]	m	6	6	$12^2$	$\sqrt{3}(5 + 11/\sqrt{5})^{1/2}$	[41 $\bar{2}$ $\bar{2}$ 21]	[ $\bar{2}$ 2 $\bar{4}$ 1 $\bar{1}$ 2]	$(-11 + 5\sqrt{5})/2$

As  $\text{tg } \theta_1 = \text{tg } \theta_2$  in the plane orthogonal to the threefold axis [011001] all periodicity directions are strong (Fig. 2). These directions together with  $\mathbf{d}_3^{\parallel}$  form the complete set of strongly periodic directions of the rhombohedral approximant.

By taking combinations of the form  $z_1\mathbf{d}_g^1 + z_2\mathbf{d}_g^2 + z_3\mathbf{d}_g^3$  we find the set of all periodicity directions in the direct space. For instance by choosing  $z_1 \cdot z_2 \cdot z_3$  equal to  $2:3:1$ ,  $2:\bar{3}:1$ ,  $1:0:\bar{1}$ , respectively, we obtain the hyperlattice directions [111112], [121 $\bar{1}$ 1], [ $\bar{1}$ 121 $\bar{1}$ 1] which project in the physical space along the directions 1, 2, 3 (Fig. 2). These are weakly periodic directions (because they do not belong to the plane of strongly periodic directions) and generate the unit cell of the rhombohedral approximant. Combining now the  $\mathbf{d}_a$  we can find the planar periodic directions. For instance  $2\mathbf{d}_a^1 + 3\mathbf{d}_a^2 - \mathbf{d}_a^3$  is parallel to (1 $\bar{1}$ 1 $\bar{1}$ 21) which projects in the physical space along the direction 4 of figure 2, a pseudo-fivefold direction in the rhombohedral approximant.

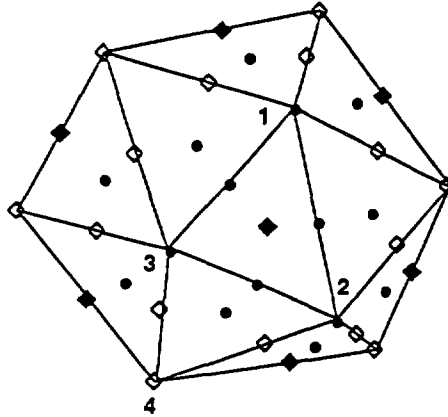


Fig. 2. — The set of the most important strong (◆), weak (●) and planar (◇) periodic directions in the rhombohedral approximant. These periodic directions are shown relatively to the axes of the icosahedral quasicrystal.

## 7. Conclusions.

This paper shows that the periodic directions in a rational approximant belong to the following three types : the weakly periodic directions, which are periodic only in the direct space ; the planar periodic directions, which are periodic only in the reciprocal space ; and the strongly periodic directions, which are periodic both in the direct and in the reciprocal space.

At first sight the set of periodic directions of a rational approximant characterize only its Bravais lattice and is more or less independent on the decoration of the Bravais lattice. This happens in ordinary crystals, but the rational approximants of the quasicrystals have a special kind of local order, which strengthens the correlation between the Bravais lattice and its decoration (a consequence of this correlation is the fact that the periods of a rational approximant cannot take any values).

The set of periodic directions is important for the identification of the rational approximant in the case where the lattice constants are large and this identification is difficult. Indeed, planar periodic and strongly periodic directions can be easily identified in the electron diffraction patterns, because the diffraction peaks are disposed in line, without zigzags, along these directions. The weakly periodic directions are orthogonal to well defined planes in the reciprocal space.

The properties of the periodic directions in rational approximants with respect to channelling were also discussed in this paper. In rational approximants there always are rows and channels parallel to weakly or strongly periodic directions and atomic planes stack orthogonally to planar or strongly periodic directions. The existence of these channelling properties has already been reported for quasicrystals in which all quasiperiodic directions are strong (this has been specified in Sect. 4), although not periodic [8, 9]. Ion channelling experiments and high resolution electron microscopy may be used for determining the set of periodic directions and identifying the rational approximants.

Planar periodic directions may be involved in the description of the stacking faults, partial dislocations, grain and twin boundaries for the rational approximants and also in the mechanisms of phase transitions between the quasicrystals and their rational approximants (see also Ref. [15]).

The importance of the strongly periodic directions lie on their stability with respect to the tilt of the strip ; we can continuously change the slopes of the strip, passing through periodic and quasiperiodic structures which have exactly the same set of strongly periodic directions. We recognize here a similar behaviour as in the case of the Schur rotations [15, 22], which continuously generate periodic and quasiperiodic structures which have a common maximal point symmetry subgroup.

Finally, some common arithmetic properties of the icosahedral modules  $P$ ,  $F$ , and  $I$ , were found. The set of all the module directions can be divided into compatibility classes which are indexed by the set of square-free numbers of the form  $5x^2 - y^2$ , with  $x, y \in \mathbb{Z}$ . Two module directions belonging to the same compatibility class carry point distributions which are correlated in a way defined by Theorem 6 of this paper. This fact can be applied to find low-energy grain boundaries between quasicrystalline or approximant grains (see also Ref. [27]). All the formalism of section 3 applies identically to the decagonal module, and can be generalized to all modules whose geometry is governed by quadratic irrationalities (see also Ref. [9]).

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### Appendix A.

**Proof of theorem 2 (theorem 3 has a completely analogous proof).**

Consider the transformation (see also [21]) :

$$\mathbf{x}^g = A_1 \mathbf{x}^{\parallel} + A_2 \mathbf{x}^{\perp} \quad (\text{A1})$$

$$\mathbf{x}^a = A_3 \mathbf{x}^{\parallel} + A_4 \mathbf{x}^{\perp} \quad (\text{A2})$$

where  $\mathbf{x}^{\parallel}$ ,  $\mathbf{x}^{\perp}$  are coordinates in  $P^{\parallel}$ , respectively  $P^{\perp}$  ;  $\mathbf{x}^g$ ,  $\mathbf{x}^a$  are coordinates in  $P^g$ ,  $P^a$ .

Using these coordinates, the equation of the grid space  $P^g$  is :

$$\mathbf{x}^{\perp} = D \mathbf{x}^{\parallel} \quad (\text{A3})$$

where  $D = -A_4^{-1} A_3$  is the phason strain matrix ([21, 28]) and the equation of the acceptance space  $P^a$  is :

$$\mathbf{x}^{\parallel} = -D^{\dagger} \mathbf{x}^{\perp} \quad (\text{A4})$$

where  $\dagger$  is for adjoint.

In the coordinate system  $(\mathbf{x}^{\parallel}, \mathbf{x}^{\perp})$  the homomorphism  $\mathfrak{F}^d$ , writes :

$$\mathbf{x}^d = \mathbf{x}^{\parallel} + D^{\dagger} \mathbf{x}^{\perp} \quad (\text{A5})$$

The following lemma is given without proof :

Lemma : If a vector  $(\mathbf{x}^{\parallel}, \mathbf{x}^{\perp})$  of a TP satisfies an equation of the form :

$$A^{\parallel}(\mathbf{x}^{\parallel}) = A^{\perp}(\mathbf{x}^{\perp}) \quad (\text{L1})$$

where  $A^{\parallel}, A^{\perp}$  are linear operators, in  $P^{\parallel}$ , respectively in  $P^{\perp}$  then all the vectors of the same TP satisfy the following equation :

$$A^{\parallel}(\mathbf{x}^{\parallel}) = kA^{\perp}(\mathbf{x}^{\perp}) \tag{L2}$$

where  $k$  is a real number,  $k \neq 0$  which changes from vector to vector. Conversely, if (L2) is satisfied with different nonzero  $k$ 's by all vectors in the TP, there is a vector in the TP which satisfies equation (L1).

The proof of Theorem 2 follows

- i)  $\Rightarrow$  ii)

If a direction  $\mathbf{d}^{\parallel}$  in the HTP is also in the grid space, then it satisfies equation (A3). Using the lemma, it can be found that  $\mathbf{d}^{\perp}$  satisfies the equation :

$$\mathbf{d}^{\perp} = kD\mathbf{d}^{\parallel} \quad \text{for some real } k \neq 0. \tag{A6}$$

Let us consider a plane  $W^{\parallel}$  of  $\mathcal{E}^{\parallel}$ , orthogonal to  $\mathbf{d}^{\parallel}$ , which passes through  $\mathbf{x}_0^{\parallel}$  and has the following equation

$$(\mathbf{x}^{\parallel} - \mathbf{x}_0^{\parallel}, \mathbf{d}^{\parallel}) = 0. \tag{A7}$$

To  $W^{\parallel}$  the isomorphism  $\mathfrak{I}$  associates a plane  $W^{\perp}$  in  $\mathcal{E}^{\perp}$ , orthogonal to  $\mathbf{d}^{\perp}$  and which has the following equation

$$(\mathbf{x}^{\perp} - \mathbf{x}_0^{\perp}, \mathbf{d}^{\perp}) = 0. \tag{A8}$$

The points  $\mathbf{x}^{\parallel} + D^{\dagger} \mathbf{x}^{\perp}$  obtained from the points of the plane  $W^{\parallel}$  by the homomorphism  $\mathfrak{I}^{\dagger}$  satisfy the equation of a plane which passes through  $\mathbf{x}_0^{\parallel} + D^{\dagger} \mathbf{x}_0^{\perp}$  and is orthogonal to  $\mathbf{d}^{\parallel}$ .

$$(\mathbf{x}^{\parallel} + D^{\dagger} \mathbf{x}^{\perp} - (\mathbf{x}_0^{\parallel} + D^{\dagger} \mathbf{x}_0^{\perp}), \mathbf{d}^{\parallel}) = 0 \tag{A9}$$

because of relations (A6-A8) and the fact that

$$(D^{\dagger}(\mathbf{x}^{\perp} - \mathbf{x}_0^{\perp}), \mathbf{d}^{\parallel}) = (\mathbf{x}^{\perp} - \mathbf{x}_0^{\perp}, D\mathbf{d}^{\parallel}) = (\mathbf{x}^{\perp} - \mathbf{x}_0^{\perp}, \mathbf{d}^{\perp})/k = 0 ;$$

- ii)  $\Rightarrow$  i)

If equation (A9) is valid while equations (A7) and (A8) are valid, then  $(\mathbf{x}^{\perp} - \mathbf{x}_0^{\perp}, D\mathbf{d}^{\parallel}) = 0$  while (A7) and (A8) are valid and therefore  $D\mathbf{d}^{\parallel}$  is parallel to the normal of the plane  $W^{\perp}$ , i.e. to  $\mathbf{d}^{\perp}$ . Using again the lemma there is a vector  $\mathbf{d}^{\parallel}$  of the HTP which satisfies equation (A3) and belongs to the grid space.

- i)  $\Leftrightarrow$  iii)

The points  $\mathbf{x}^{\parallel}$  on a direction  $\mathcal{D}^{\parallel}$  parallel to  $\mathbf{d}^{\parallel}$ , which passes through  $\mathbf{x}_0^{\parallel}$  are of the form  $\mathbf{x}^{\parallel} = \mathbf{x}_0^{\parallel} + \mathbf{y}^{\parallel}$ , where  $\mathbf{y}^{\parallel}$  is the projection onto  $P^{\parallel}$  of some vector in the HTP corresponding to  $\mathbf{d}^{\parallel}$ . The isomorphism  $\mathfrak{I}$  put this direction into correspondence with the direction  $\mathcal{D}^{\perp}$  in  $P^{\perp}$  :  $\mathbf{x}^{\perp} = \mathbf{x}_0^{\perp} + \mathbf{y}^{\perp}$ . The homomorphism  $\mathfrak{I}^{\dagger}$  which is described by relation (A2) transforms the points on the line  $\mathcal{D}^{\parallel}$  onto :

$$\mathbf{x}^{\perp} = A_4(\mathbf{x}_0^{\perp} - D\mathbf{x}_0^{\parallel}) + A_4(\mathbf{y}^{\perp} - D\mathbf{y}^{\parallel}). \tag{A10}$$

Equation (A10) represents the equation of a direction in  $P^{\perp}$  if  $\mathbf{y}^{\perp}$  is parallel to  $D\mathbf{y}^{\parallel}$  for all the points of the HTP corresponding to  $\mathbf{d}^{\parallel}$ , i.e., using lemma, if the above HTP has a 1-D intersection with the grid space.

## Appendix B.

### Proof of theorem 5.

If equation (10a) is fulfilled then relation (4) is fulfilled with  $p = 1$  and  $q = 0$ . In this case, the ratio of the periods along  $\mathbf{d}_1^\parallel$ ,  $\mathbf{d}_2^\parallel$ , respectively must be (use (2) and (6)) :

$$\left( \frac{P(\mathbf{d}_1)}{P(\mathbf{d}_2)} \right)^+ = \left( \frac{\sqrt{5}x(\mathbf{d}_1) + y(\mathbf{d}_1)}{\sqrt{5}x(\mathbf{d}_2) + y(\mathbf{d}_2)} \right)^{1/2} = \left( \frac{\sqrt{5}x(\mathbf{d}_1) - y(\mathbf{d}_1)}{\sqrt{5}x(\mathbf{d}_2) - y(\mathbf{d}_2)} \right)^{1/2} = \left( \frac{n(\mathbf{d}_1)}{n(\mathbf{d}_2)} \right)^{1/2} \quad (\text{B1})$$

Of course there is a countable set of other pairs of periods on  $\mathbf{d}_1^\parallel$ ,  $\mathbf{d}_2^\parallel$  compatible with relation (10a) ; all these pairs are obtained by applying the operators  $T_{p,q}$  to  $\mathbf{d}_1$ ,  $\mathbf{d}_2$ . Using once again relation (2) we obtain

$$\left( \frac{P(p, q; \mathbf{d}_1)}{P(p, q; \mathbf{d}_2)} \right)^+ = \frac{k(p, q; \mathbf{d}_2)}{k(p, q; \mathbf{d}_1)} \left( \frac{n(\mathbf{d}_1)}{n(\mathbf{d}_2)} \right)^{1/2} \quad (\text{B2})$$

To see what happens when (10b) is fulfilled, first note that in (3),  $\text{tg } \theta(0, 1; \mathbf{d}) = -\text{tg } \theta(\mathbf{d})$  and, using (2),  $P(0, 1; \mathbf{d})/P(\mathbf{d}) = \sqrt{5}/k(0, 1; \mathbf{d})$ . Reciprocally  $P(\mathbf{d})/P(0, 1; \mathbf{d}) = \sqrt{5}/k(0, 1; \mathbf{d}^-)$ , where  $\mathbf{d}^-$  is the primitive hyperlattice vector collinear with  $T_{0,1}\mathbf{d}$ . This shows that  $k(0, 1; \mathbf{d})k(0, 1; \mathbf{d}^-) = 5$  and  $P(0, 1; \mathbf{d})/P(\mathbf{d}) = \sqrt{5}$  or  $1/\sqrt{5}$ . As a consequence, if (10b) is fulfilled, the ratios (B1), (B2) are multiplied by a factor  $\sqrt{5}$  or  $1/\sqrt{5}$ .

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- [17] Particular cases of the relations (2), (3) can be found in many places ; see reference [16] and Mukhopadhyay N. K., Ishihara K. N., Ranghanatan S. and Chattopadhyay K., *Acta Metall.* **39** (1991) 1151 ; Baake M., Joseph D. and Kramer P., *J. Phys. A* (1990) L961 ; The set of all numbers of the form  $\pm (p - q\sqrt{5})/(p + q\sqrt{5})$  form a multiplicative group in the field  $\mathbb{Q}(\sqrt{5})$  and contains as a subgroup all the even powers of the golden number  $\tau = (1 + \sqrt{5})/2$ . This group has some other interesting properties, which are not given here. Note only that

relation (4) demands finding the squares in this group, and the solution is a condition on the norm  $p^2 - 5q^2$  which must be a square. A useful reference for the algebra of  $\mathbb{Q}(\sqrt{5})$  is Dodd F. W., *Number Theory in the Quadratic Field with Golden Section Unit* (Polygonal Publishing House, 1983).

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