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► **To cite this version:**

A. Katz, M. Duneau. QUASIPERIODIC STRUCTURES OBTAINED BY THE PROJECTION METHOD. Journal de Physique Colloques, 1986, 47 (C3), pp.C3-103-C3-112. 10.1051/jphyscol:1986310 . jpa-00225721

HAL Id: jpa-00225721

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Submitted on 4 Feb 2008

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QUASIPERIODIC STRUCTURES OBTAINED BY THE PROJECTION METHOD

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Résumé - Les propriétés générales des structures quasi-périodiques obtenues par la méthode de projection sont présentées en vue d'un modèle structural des cristaux aperiodiques du type Al-Mn. On étudie particulièrement les environnements locaux, les projections à 2 dimensions de ces structures et leur transformée de Fourier.

Abstract - The general properties of quasiperiodic structures obtained by the projection method are given in view of a structural model of aperiodic crystals of type Al-Mn. The local environments, the 2-dimensional projections and the Fourier transform of these structures are particularly examined.

1 INTRODUCTION

This talk deals with some specific features of quasiperiodic tilings or patterns obtained by the projection method.

Non periodic tilings were first introduced in connection with problems of mathematical logics but the invention by R. Penrose of his well known aperiodic tilings of the plane initiated the study of the geometrical properties of these patterns with the pionnering works of R. Penrose [1], J. Conway (see [3]) and N. G. de Bruijn [2] (see the beautiful survey by M. Gardner [3]). The possible implications of these structures for solid state physics were mentioned by A. L. Mackay [4] and Mosseri and Sadoc [5]. A 3-dimensional generalization of the Penrose tilings (using two rhombohedra instead of two rhombs) was devised by R. Ammann and theoretically described by P. Kramer and R. Neri [6] and P. Kramer [7] using the de Bruijn's framework. The spectral properties of the Penrose patterns were first observed by A. L. Mackay, using optical methods. The presence of sharp Bragg peaks in the diffraction patterns is now identified [8,9,10,11] as the expression of quasiperiodicity : the Fourier transform of the measure defined as the sum of Dirac deltas at all vertices of the tiling, is a sum of weighted Dirac measures carried by a \mathbb{Z} -module.

The experimental discovery of icosahedral symmetry together with some kind of long range spatial order in quenched Al-Mn alloys by D. Shechtman et al. [12] aroused a great interest among theorists, as well on the structural problem, as on stability questions which will not be discussed here.

The projection method, already introduced in de Bruijn [2] and developed by P.A. Kalugin et al. [10], V. Elser [11] and us [8,9] is now widespread so that we shall only give a short recall of this method in one dimension and then consider three specific questions arising in the 3-dimensional icosahedral patterns, namely the description of local environments, the relation between the 3-dim patterns and their various 2-dimensional projections, and the computation of the Fourier transform.

2 THE ONE-DIMENSIONAL MODEL

Let us begin by a brief description of the projection method in the 1-dimensional case (Fig.1) : consider the plane \mathbb{R}^2 , the square lattice \mathbb{Z}^2 and a line E to be tiled. A strip is obtained by shifting the unit square K along E . Then, for almost all positions of the line, this strip contains a unique broken line (made of edges of the lattice), which joins exactly all the vertices inside the strip. The orthogonal projection of this line on E gives a tiling, the two tiles a and b being the projections of the vertical and horizontal edges of the unit square K .

This construction depends basically on the three following parameters :

1) The choice of the unit square to build the strip implies that the corresponding tiling involves only two tiles. Actually, if the unit square is replaced by any other unit cell of \mathbb{Z}^2 , new tilings involving the projections of the two edges of this cell are obtained. This is closely related to self-similarity properties. However, the projection method should not be restricted to these tilings since more general strips also generate tilings involving a finite number of tiles and a finite number of local environments.

2) Consider now the slope of the line E with respect to the canonical basis of \mathbb{R}^2 . One easily checks that the tiling is periodic if and only if this slope is a rational number. In the case of the standard tiling, the slope is just the ratio of the relative frequency of the two tiles, and this ratio is rational only for a periodic tiling.

3) Given an irrational slope, consider a small translation of the strip. Then, each time a point leaves the strip, another point enters the strip. These two points are the vertices of a diagonal of some square in the lattice, in such a way that the broken line "jumps" from one side of the square to the other. This is the only elementary process which allows to generate all tilings. Of course, any non trivial translation of the strip implies infinitely many such jumps.

An important property of these patterns is the local isomorphism property, introduced as a property of Penrose tilings, which asserts that any finite patch of tiles that belongs to a tiling appears infinitely many times in any tiling defined through a strip with the same irrational slope. Such a finite patch of tiles in a given tiling is the projection of a finite broken line, the projection of which on E' is strictly smaller than the projection of the whole strip. Then there exists a non empty open set of translations in E' that keep the projection of the finite broken line inside the strip. Since the projection of \mathbb{Z}^2 on E' is dense, there are infinitely many translations of \mathbb{Z}^2 which map the finite broken line inside the strip, thus giving infinitely many copies of the initial patch of tiles. One can show along the same lines that any finite patch of tiles that appears in a tiling appears in all tilings with the same slope.

There are interesting questions concerning the mean distance between copies of a given patch. The density of the copies of a patch depends on arithmetical properties of the slope.

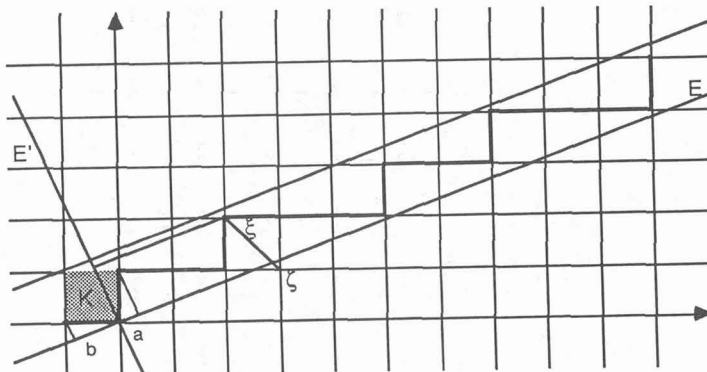


Fig. 1 : The projection method in 1 dim : the line E is tiled by the projection of the broken line contained in the strip $S=E+K$ where K is the unit square of \mathbb{Z}^2 .

As can be seen in Fig. 1, the set of translations corresponding to the broken line limited by the origin and ξ , is closely related to the approximation of the slope given by ζ . For algebraic numbers, the mean distance between two copies is proportionnal to the size of the patch, but for Liouville numbers, this distance can grow arbitrarily quickly.

Finally, let us describe the computation of the Fourier transform of the measure defined by putting one Dirac delta at each vertex of the tiling (Fig.2). This measure is obtained in three steps : take the square lattice of Dirac deltas in the plane, multiply by the characteristic function of the strip, and then project on the line. The Fourier transform is obtained by carrying out the corresponding steps in the reciprocal space. The first one yields the Fourier transform of the square lattice, which is the reciprocal square lattice of Dirac deltas. The second step is the convolution by the Fourier transform of the characteristic function of the strip, the computation of which is straightforward since it is a product : in the direction E^* dual to the direction of the strip, this Fourier transform is a Dirac delta $\delta(k)$ and in the orthogonal direction E'^* , it is the smooth function $\sin(\pi k')/\pi k'$ (up to a normalisation). The convolution amounts to translate a copy of this Fourier transform at each point of the reciprocal lattice. Finally, the Fourier image of the projection is merely the restriction to the line E^* (Fig.2).

The most important point is that the Fourier transform thus obtained is a sum of weighted Dirac deltas, carried by a \mathbb{Z} -module given by the projection of the whole reciprocal lattice \mathbb{Z}^2 on E^* . The second point is that a translation of the strip only changes the phases of Dirac deltas in such a way that all the tilings associated with the same irrational slope yield the same diffraction patterns, as far as only intensities are measured.

Notice finally that, although the support of the Fourier transform is a dense set, the intense peaks correspond to vertices which are close to the line E^* , and that the set of peaks with an intensity greater than any positive threshold is always discrete.

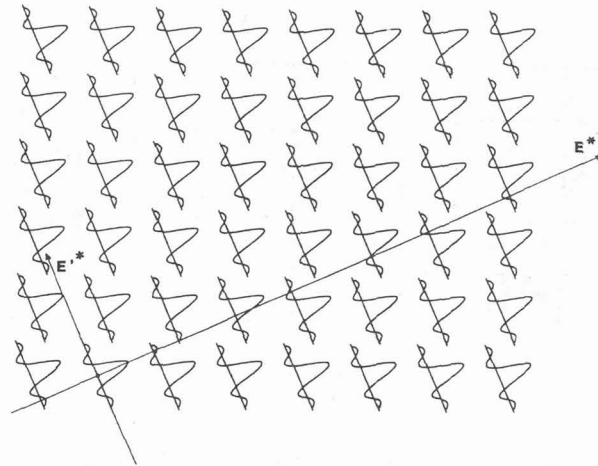


Fig. 2 : The Fourier Transform of the 1-dimensional tiling is given by the section $k=0$ of the distribution defined by the convolution of $\delta(k) \cdot \sin(\pi k')/\pi k'$ with the reciprocal lattice.

3 ICOSAHEDRAL PATTERNS IN \mathbb{R}^3

The projection method can be worked out in view of the icosahedral symmetry. The simplest construction involves a projection from \mathbb{R}^6 where an orthogonal representation of the icosahedral group is obtained by "lifting" its action on the 12 vertices of an icosahedron to the 12 oriented axes of \mathbb{R}^6 . Then \mathbb{R}^6 falls into two invariant 3-spaces, E (the space of the tiling) and E' endowed with non-equivalent representations.

Let $\{e_1, e_2, e_3, e_4, e_5, e_6\}$ denotes the standard orthonormal basis of \mathbb{R}^6 and let π and π' denote the orthogonal projectors on E and E' . Then, the 6 vectors e_1, \dots, e_6 project on respectively e_1, \dots, e_6 in E , and e'_1, \dots, e'_6 in E' in such a way that $\pm e_1, \dots, \pm e_6$ and $\pm e'_1, \dots, \pm e'_6$ point to the 12 vertices of a regular icosahedron (Fig.3).

The unit cube $\gamma_6 = \{ \sum \xi_i e_i \mid 0 < \xi_i < 1 \}$ of \mathbb{R}^6 projects in E and in E' on a "rhombic triacontahedron", a convex polyhedron with 32 vertices, 30 identical facets and 60 edges. The vertices correspond to the 12 vertices of an icosahedron and the 20 vertices of a dodecahedron with the same orientation.

The 20 different 3-facets of \mathbb{Z}^6 fall in E (and E') on only 2 different rhombohedra, a flat one and a thick one, with the same facets (with angles $\text{Atn}(2) = 63^\circ 26'$, $\pi - \text{Atn}(2)$) and edge $1/\sqrt{2}$, each one occurring in 10 different orientations. These are the rhombohedra considered by A.L. Mackay [4], P. Kramer and R. Neri [6] and introduced by R. Ammann.

Since e_1, \dots, e_6 and e'_1, \dots, e'_6 are rationally independant, the projections π and π' have a one to one restriction to \mathbb{Z}^6 . The images $L = \pi(\mathbb{Z}^6)$ and $L' = \pi'(\mathbb{Z}^6)$ are \mathbb{Z} -modules generated respectively by e_1, \dots, e_6 and e'_1, \dots, e'_6 which are dense and homogeneous in E and E' . A natural isomorphism φ of L onto L' is defined by $\varphi(e_i) = e'_i$, which amounts to lift L to \mathbb{Z}^6 and to project on L' (of course this isomorphism does not extend to E).

A 3-dimensional Penrose tiling is obtained with the strip defined by shifting the unit cube γ_6 along $E : S = E + \gamma_6 = \{\xi + \zeta \mid \xi \in E, \zeta \in \gamma_6\}$. The lattice points of Z^6 which fall inside the strip, i.e. $S \cap Z^6$, all belong to a 3-dimensional manifold made of the 3-facets of Z^6 which are entirely contained in S . The projection of this manifold on E yields a tiling by means of the two rhombohedra, the vertices of which are given by the projection $\pi(S \cap Z^6)$ in E .

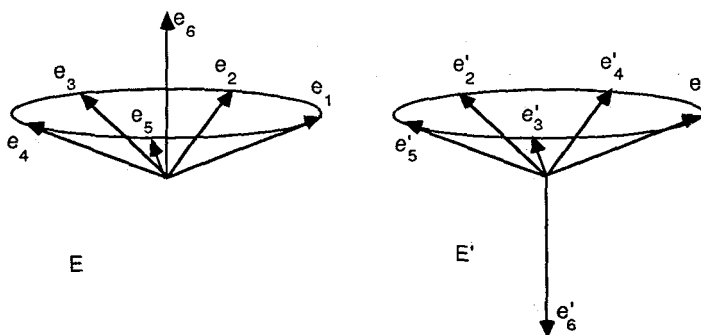


Fig. 3 : The projections of the standard orthonormal basis of \mathbb{R}^6 in E and E' .

This set is in a one to one correspondance, by means of ϕ with the other projection $\pi'(S \cap Z^6)$ in E' , so that the set of vertices is just the image by ϕ^{-1} of the points of L' which fall inside the triacontahedron in E' .

As in the 1-dimensional case we obtain different tilings when the strip S is translated in \mathbb{R}^6 . For $\alpha \in \mathbb{R}^6$, the strip $S_\alpha = S + \alpha$ yields the tiling $\pi(S_\alpha \cap Z^6)$ which is non isomorphic to the initial one if $\alpha \notin L'$. Notice that if $\alpha \in L'$, the new tiling is just a translate of the initial one by $\phi^{-1}(\alpha)$. As mentioned above, the tiling is completely specified by the projection of S_α in E' , which involves a translation of the triacontahedron by $\pi'(\alpha)$. Thus the set of non isomorphic tilings can be labelled by the quotient set E'/L' , which is uncountable.

An important generalization of these tilings is obtained by replacing the triacontahedron with an arbitrary bounded open set K of E' . The corresponding strip is then $\pi^{-1}(K)$, the intersection of which with Z^6 specifies the vertices of the new pattern by projection in E . A general argument insures that the pattern is discrete as soon as the projection K of the strip in E' is bounded. The mean density of such a pattern is simply equal to the volume of K : actually, the number of points in a finite region B of E is roughly equal to the number of points of Z^6 in the subset $B \times K$ of $E \times E' = \mathbb{R}^6$. In such a situation, the pattern will still involve only a finite number of local environments. This choice allows to raise the problem of dense packings with icosahedral symmetry : given a minimal distance d between vertices in E , find the maximal sets K in E' , with icosahedral symmetry, such that the corresponding patterns in E do not show smaller distances than d . This question arises in connection with the structure of the quasicrystal, whatever the unit (atoms or Mackay's icosahedra).

Let us mention a possible generalization which will not be discussed in this paper : the strip can be defined by means of a 3-dimensional subspace $E^{(1)}$, i.e. $S = E^{(1)} + K$, different from the 3-dimensional physical space $E^{(2)}$. Besides, the direction of the projection on $E^{(2)}$ can be chosen independently. $E^{(1)}$ controls the relative frequencies of local patterns and the periodicity properties of the tiling. For instance, if $E^{(1)}$ is a lattice subspace and $E^{(2)} = E$, a

periodic tiling of E by means of the above two rhombohedra is obtained. When $E^{(1)}$ tends to E , the periodic tilings have larger and larger fundamental cells, and "converge" to the quasiperiodic tiling. Such commensurate approximations seem to be connected with crystal phases (α -AlMnSi) close to the quasicrystal [14,15,16,17].

4 LOCAL PATTERNS OF THE ICOSAHEDRAL TILINGS

The local structure of the tilings can be described by means of all possible local environments of vertices in terms of rhombohedra, together with their relative frequencies. Another possible description, which applies to general patterns, is that of all nearest-neighbour configurations around the vertices. Both descriptions can be obtained using the same arguments which we present below in the case of a tiling. Let $S = E + \gamma_6$ be the strip and let $K = \pi'(S)$ denote the triacontahedron. For any vertex $x = \pi(\xi)$, where $\xi \in S \cap \mathbb{Z}^6$ and $x' = \pi'(\xi) \in K$, the rhombohedron spanned by e_i, e_j, e_k is attached to x iff the corresponding one spanned by e'_i, e'_j, e'_k and attached to x' in E' , is entirely contained in K . The set of such points x' in K can be seen to be the intersection of L' with a "complementary" rhombohedra spanned by e'_i, e'_m, e'_n , where $\{i, m, n\}$ is the complement of $\{i, j, k\}$ in $\{1, 2, 3, 4, 5, 6\}$ (Fig.4). For the same reasons, the relative frequency of a given rhombohedron is proportional to the volume of the "complementary" rhombohedron of its image in E' : the relative frequency is $\tau^{-1}/10$ for each orientation of the thick rhombohedron, and $\tau^{-2}/10$ for those of the thin one.

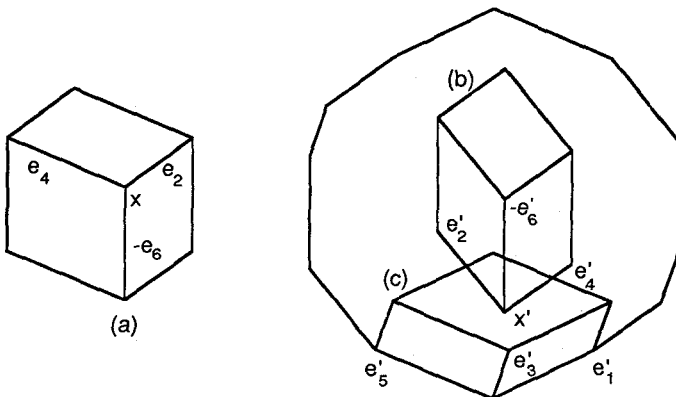


Fig. 4 : The rhombohedron (a) spanned by e_2, e_4 and $-e_6$ is attached at x , iff the corresponding rhombohedron (b) spanned by e'_2, e'_4 and $-e'_6$ at x' is entirely contained in the triacontahedron. The acceptance domain for x' is the rhombohedron (c) spanned by e'_1, e'_3 and e'_5 .

A partition of K is induced by the projection of the 160 different 3-facets of γ_6 . The cells of this partition are associated to all possible environments of rhombohedra around the vertices of the tiling and the relative frequency of each arrangement is given by the quotient of the volume of the corresponding cell by the volume of the whole triacontahedron. It turns out that, up to rotations and inversion, there are only 24 such possible vertex neighbourhoods,

which involve from four to twenty rhombohedra. One can see that a true tiling of E is actually obtained since for all possible neighbourhood the whole surrounding space is filled with non-overlapping rhombohedra. The simplest vertex neighbourhood consists of two thick and two thin rhombohedra, the union of which is a rhombic dodecahedron, which holds for the fraction τ^{-3} of all the vertices. Furthermore, the closure of the corresponding cells contains the boundary of the triacontahedron, which implies that the elementary process involved in a translation of the strip concerns generically only this type of vertex : what happens is merely a "jump" of the internal vertex of the rhombic dodecahedron from one position to the unique other possible position (notice the similarity with the one-dimensional case described above). The central cell of this partition corresponds to vertices surrounded by a 20-pronged star of thick rhombohedra, which have a relative frequency of τ^{-9} .

5 PROJECTIONS OF THE ICOSAHEDRAL PATTERNS

The micrographs of the quasicrystals are known to show discrete patterns of bright spots (see for instance R. Portier). Although their relation with the real structure is not clearly understood, it is worthwhile checking if the icosahedral patterns obtained by projection methods can produce such discrete projections from a purely geometric point of view. This is indeed the case as we show in this section.

The \mathbf{Z} -modules $\mathbf{L}=\pi(\mathbf{Z}^6)$ in E and $\mathbf{L}'=\pi'(\mathbf{Z}^6)$ in E' are generated by the projections e_1, \dots, e_6 , and e'_1, \dots, e'_6 respectively. The natural generalizations of the lattice directions and lattice planes of classical crystallography, are the quasi-lattice directions and quasi-lattice planes defined as the subspaces of E (or E'), spanned by one or two (\mathbf{R} -independent) vectors of \mathbf{L} (or \mathbf{L}'). For instance, if $d=\sum \eta_i e_i \in \mathbf{L}$ ($\eta_i \in \mathbf{Z}$ for $i=1, \dots, 6$), the corresponding quasi-lattice direction is just the line $D=\mathbf{R}.d$ of E spanned by d .

Now, using the natural isomorphism ϕ of \mathbf{L} onto \mathbf{L}' , given by $\phi(e_i)=e'_i$, we can map any quasi-lattice direction D of E , spanned by $d=\sum \eta_i e_i$, to the quasi-lattice direction D' of E' spanned by $d'=\sum \eta_i e'_i$. One easily checks that $d+d'=\sum \eta_i \xi_i$ and $\sqrt{5}(d-d')$ belong to \mathbf{Z}^6 . Thus the direct sum $W=D \oplus D'$ is a lattice plane of \mathbf{Z}^6 which projects onto D in E and onto D' in E' . Furthermore, the lattice points which fall on D or on D' , all belong to the 2-dim lattice $W \cap \mathbf{Z}^6$, i.e. $\pi^{-1}(D \cap \mathbf{L})=W \cap \mathbf{Z}^6$: if $x \in D \cap \mathbf{L}$, x is the projection of a unique point $\xi \in \mathbf{Z}^6$; if $x'=\phi(x)$ then $x' \in D'$ so that $\xi=x+x' \in W \cap \mathbf{Z}^6$ and projects on x . Similarly, $\pi'^{-1}(D' \cap \mathbf{L}')=W \cap \mathbf{Z}^6$.

If D is a quasi-lattice direction of E , the orthogonal complement of D in E is a quasi-lattice plane P and the orthogonal complement $V=W^\perp$ of $W=D \oplus D'$, is a lattice 4-plane of \mathbf{Z}^6 such that $P=\pi(V)$ and $P'=\pi'(V)$. One shows in a similar way that $\pi^{-1}(P \cap \mathbf{L})=\pi^{-1}(P' \cap \mathbf{L}')=V \cap \mathbf{Z}^6$: the lattice points which fall on P or P' all belong to the 4-dim lattice $V \cap \mathbf{Z}^6$.

Consider the pattern $\pi(S \cap \mathbf{Z}^6)$, associated to the strip $S=\pi^{-1}(K)$, where K is a bounded subset of E' . Let P be the quasi-lattice plane of E on which we want to project this pattern and let $V=P \oplus P'$ be the corresponding lattice 4-plane. Let D be the quasi-lattice direction of E orthogonal to P and let $W=D \oplus D'$ denote the corresponding lattice 2-plane. The projections of \mathbf{Z}^6 on P and P' are dense \mathbf{Z} -modules which can be obtained by projecting the lattice $\mathbf{L}_V=\pi_V(\mathbf{Z}^6)$, where π_V is the orthogonal projector on $V=P \oplus P'$. \mathbf{L}_V is in general a lattice with a basis, the translation group of which is $V \cap \mathbf{Z}^6$. One can check that $P \cap \mathbf{L}_V=\{0\}$ and $P' \cap \mathbf{L}_V=\{0\}$ so that the projections of \mathbf{L}_V on P and P' are one to one.

The projection of the pattern on P is given by $\pi_P(S \cap Z^6)$, where π_P is the orthogonal projector on P . If $x = \pi_P(\xi_1) = \pi_P(\xi_2)$ is the projection of two points $\xi_1, \xi_2 \in S \cap Z^6$, then $x_1 = \pi(\xi_1)$ and $x_2 = \pi(\xi_2)$ are two vertices of the pattern such that $x_1 - x_2 \in D$. Now, $x'_1 = \phi(x_1)$ and $x'_2 = \phi(x_2)$ belong to K and satisfy $x'_1 - x'_2 \in D'$ so that $x' = \pi_{P'}(\xi_1) = \pi_{P'}(\xi_2)$ belongs to $\pi_{P'}(S \cap Z^6)$, where $\pi_{P'}$ is the orthogonal projector on P' (Fig. 5).

For any point x' in the Z -module $\pi_{P'}(Z^6)$, the line $x' + D'$ has a dense intersection with L' so that if x' is in $\pi_{P'}(S \cap Z^6)$, there are infinitely many points in $K \cap L'$ which fall on x' . Finally, any point x in the projected pattern is the projection of infinitely many points of the original pattern, which correspond in E' to the intersection of the line $x' + D'$ with $K \cap L'$. The length of this interval is clearly proportional to the frequency of points of the original pattern above x . This property could be used to check or even to derive the shape of K from the images obtained by high resolution electron microscopy, as mentioned by R. Portier in his conference (this issue).

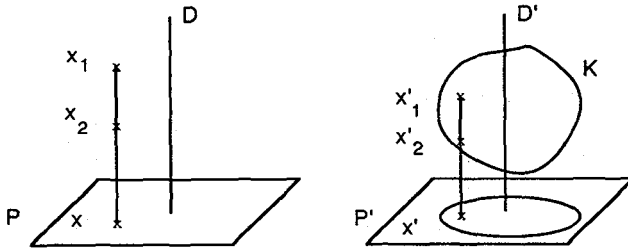


Fig. 5 : If x_1 and x_2 belong to the pattern in E and project on x in P , then x'_1 and x'_2 belong to K and project on x' in P' . The density of points of the pattern above x is proportional to the length of the intersection of the line $x' + D'$ with K .

It follows from the above description that the projected pattern $\pi_P(S \cap Z^6)$ can be obtained directly from a strip method in $V = P \oplus P'$: the lattice to be considered is $L_V = \pi_V(Z^6)$ and the strip is defined by $S_V = P + \pi_V(S)$. The projected pattern is given by $\pi_P(S_V \cap L_V)$. Since the projection of L_V on P and P' is one to one, the projected pattern is in a one to one correspondance with the other projection in P' . Moreover, the general argument given above insures that this pattern is discrete. Its density can easily be deduced from the density of the lattice L_V and the surface of $\pi_{P'}(K)$.

In a similar way, one can see that the projection of the pattern on any quasi-lattice direction D is discrete, and can be directly obtained from a strip method in the 2-dimensional lattice plane $W = D \oplus D'$ with the lattice $L_W = \pi_W(Z^6)$ and the strip $S_W = D + \pi_W(S)$, where π_W is the orthogonal projector on W .

6 FOURIER TRANSFORM

The most striking property of quasicrystals [12] is their ability to produce sharp Bragg peaks by diffraction while the electron diffraction patterns reveal the symmetry of the icosahedral group, which is incompatible with translation invariance. As we show below, the strip method gives an evidence of this fact by a straightforward calculation, derived independently in [10] and [11].

The mathematical underlying feature of this property of the icosahedral patterns is the quasiperiodicity of the associated measures. A measure m on \mathbb{R}^n is said to be quasiperiodic iff its Fourier transform m^* is a linear combination of Dirac measures carried by a \mathbf{Z} -module spanned by finitely many generators of \mathbb{R}^n .

The measure m associated to the pattern is defined by a Dirac delta at each vertex of the pattern, i.e. $m = \sum_{\xi \in \Xi} \delta_{\pi(\xi)}$, where $\Xi = S \cap \mathbf{Z}^6$. The Fourier transform of m is formally given by $m^*(k) = \sum_{\xi \in \Xi} e^{2i\pi k \cdot \pi(\xi)}$. Consider now the measure in \mathbb{R}^6 defined by $\mu = \sum_{\xi \in \Xi} \delta_{\xi}$; then $\mu^*(\kappa) = \sum_{\xi \in \Xi} e^{2i\pi \kappa \cdot \xi}$. Using the orthogonal decomposition $\xi = (x, x')$ and $\kappa = (k, k')$ of \mathbb{R}^6 and its dual space into $E \oplus E'$ and $E^* \oplus E'^*$, we see that $m^*(k) = \mu^*(k, 0)$, so that m^* is a section of μ^* .

If χ_S denotes the characteristic function of the strip S in \mathbb{R}^6 , $\mu = \chi_S \cdot \sum_{\xi \in \mathbf{Z}^6} \delta_{\xi}$ and consequently, the Fourier transform μ^* is given by the convolution $\mu^* = (\chi_S^*) * (\sum_{\kappa \in \mathbf{Z}^6} \delta_{\kappa})$, i.e. $\mu^*(x) = \sum_{\lambda \in \mathbf{Z}^6} \chi_S^*(x - \lambda)$ where χ_S^* is the Fourier transform of χ_S in \mathbb{R}^6 . Since $S = E + K$, the characteristic function satisfies $\chi_S(x, x') = \chi_K(x')$ where χ_K is the characteristic function of K in E' . Therefore, $\chi_S^*(k, k') = \delta(k)$. $\chi_K^*(k')$ and the Fourier transform μ^* is given by $\mu^*(k, k') = \sum_{\lambda \in \mathbf{Z}^6} \chi_K^*(k' - l')$ where $\lambda = (l, l')$ is the decomposition of λ in $E^* \oplus E'^*$. Finally, the Fourier transform m^* is given by $m^*(k) = \sum_{\lambda \in \mathbf{Z}^6} \chi_K^*(l')$ $\delta(k - l)$.

We see that m^* is a sum of weighted Dirac measures carried by the \mathbf{Z} -module L , which implies its quasiperiodicity, according to the above definition. Since the projection of \mathbf{Z}^6 on L is one to one, the amplitude of the Dirac measure at $k = \pi(\kappa)$ is simply given by $\chi_K^*(k')$. If K is bounded, χ_K^* tends to 0 at infinity so that the most intense peaks are associated to points $\kappa \in \mathbf{Z}^6$ which are close to E , i.e. to approximations of E by the lattice points of \mathbf{Z}^6 . Actually, in any finite domain of the Fourier space, there are finitely many points with an absolute value of the amplitude above any given positive threshold.

Assume now that the previous strip $S = \pi^{-1}(K)$ is translated by $\alpha \in E'$. One easily checks that the Fourier transform of the new pattern is given by $m^*_\alpha(k) = \sum_{\lambda \in \mathbf{Z}^6} e^{2i\pi \alpha \cdot l'} \cdot \chi_K^*(l') \cdot \delta(k - l)$. In other words, only the phases of the different weighted Dirac measures are changed by a translation, and from a "diffractive" point of view, all the patterns associated to a given strip, up to a translation, give rise to identical diffraction patterns, as far as only intensities are measured.

The computation of the Fourier transform m^* in different quasi-lattice planes of E^* is given in [9]. Let us just mention that if P is such a plane, the restriction of m^* to P is simply obtained by restricting the summation on \mathbf{Z}^6 to the lattice 4-plane $V = P \oplus P'$, i.e. to the sub-lattice $V \cap \mathbf{Z}^6$.

The computation of the Fourier transform on a quasi-lattice direction is particularly simple since it reduces to a 2-dimensional construction : If D is a quasi-lattice direction of E^* spanned by d , the Dirac measures on D are associated to the lattice points of $W = D \oplus D'$. The corresponding weights $\chi_K^*(-k')$ of the Fourier transform are related to the decomposition $\kappa = (k, k')$ of $\kappa \in W \cap \mathbf{Z}^6$ in D and D' . Thus, the highest weights refer to the best approximations of D by the lattice points of the 2-dimensional lattice $W \cap \mathbf{Z}^6$.

Consider for instance the Fourier transform on a 5-fold axis such as the line D generated by $d = e_6$, which appears in a plane orthogonal to a 2-fold axis. An orthogonal basis of $W \cap \mathbf{Z}^6$ is given by $\omega_1 = e_6$ and $\omega_2 = e_1 + e_2 + e_3 + e_4 + e_5$ so that $d + d' = \omega_1$ and $\sqrt{5}(d - d') = \omega_2$. Then $d = (\sqrt{5} \omega_1 + \omega_2) / (2\sqrt{5})$ and $d' = (\sqrt{5} \omega_1 - \omega_2) / (2\sqrt{5})$ and the slope of D is $1/\sqrt{5}$. A generic point $\kappa = n_1 \omega_1 + n_2 \omega_2$ of $W \cap \mathbf{Z}^6$ projects on $k = (n_1 + n_2 \sqrt{5})e_6$ on D and on $k' = (n_1 - n_2 \sqrt{5})e'_6$ on D' . The construction of the Fourier transform is then straightforward. Of particular interest are the most intense peaks which correspond to convergents and which can be used for the indexation of

the diffraction pattern. The continued fraction of $\sqrt{5}$ is $\{2,4,4,4,4,\dots\}$ so that the convergents p_n/q_n are given by the recursion formula $p_{n+2}=4p_{n+1}+p_n$ and similarly $q_{n+2}=4q_{n+1}+q_n$, with the initial conditions $p_0=2, p_1=9$ and $q_0=1, q_1=4$. The first terms of $\{p_n\}$ are $\{2,9,38,161,\dots\}$, whereas those of $\{q_n\}$ are $\{1,4,17,72,\dots\}$. The corresponding Dirac measures are located at $k_n=(p_n+\sqrt{5}q_n)e_6$, and the amplitudes are given by $\chi^*_K(-k'_n)$ with $k'_n=(p_n-\sqrt{5}q_n)e'_6$.

The lattice parameter a for the cubic lattice in \mathbf{R}^6 can be derived using the following scaled Fourier transforms. The corresponding strip is now $a \cdot S = E + a \cdot K$ where K is the previous unscaled volume in E' and $a \cdot K$ denotes the homotetic of K . Then the Fourier transform of $\chi_{a,S}$ is given by $\chi^*_{a,S}(k,k') = a^{-3} \cdot \chi^*_K(a \cdot k') \cdot \delta(k)$. The Fourier transform of the lattice is $a^{-6} \sum_{\lambda \in Z^6} \delta_{a^{-1}\lambda}$ and finally we obtain :

$$m^*(k) = a^{-3} \sum_{\lambda \in Z^6} \chi^*_K(-l') \delta(k-l/a)$$

Notice that the generators $\{e_i\}$ of L and $\{e_i^*\}$ of L^* are respectively of norm $a/\sqrt{2}$ and $1/\sqrt{2}a$. Therefore we have the relation $|e_i| \cdot |e_i^*| = 1/2$ (or $|e_i| \cdot |e_i^*| = \pi$ for the other normalization of the Fourier transform).

The X-ray diffraction analysis given by P. A. Bancel et al. [18] indicates that the first convergent $(2+\sqrt{5})|e_i^*|$ on a 5-fold axis, (indexed (10000) by the authors) and which appears in the diffraction patterns orthogonal to a 2-fold axis, corresponds to 2.896 \AA^{-1} from which follows $|e_i^*| = a/\sqrt{2} = 4.59 \text{ \AA}$ (using the correct normalization).

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COMMENTS AFTER THE A. KATZ TALK :

M.V. JARIC.-

Question :

You have mentioned in your talk what I believe to be the "lowest order", generic, singular tilings. In analogy with the singular and exceptionally singular two-dimensional tilings, could you tell us something about the possible "higher order" singular tilings and the local rearrangements to which they belong ?

Response by A. KATZ and M. DUNEAU :

The equivalence between the projection method and the grid method is such that the singular tilings for the grid method correspond to singular positions of the triacontahedron K in the projection method. Generically, the boundary of K does not intersect the module L' . The non generic positions of K are associated to transitions between tilings. In generic transitions, points of faces of K are exchanged in such a way that in the tiling, inner points of rhombic dodecahedron jump from one position to the unique other one. Non generic transitions, which correspond to exceptional singular tilings in the grid method, occur if edges or vertices of K also intersect L' and these transitions can be decomposed in generic ones.

Question :

Are the twenty four local environment obtained by your method equivalent to the local environments determined by intersections of the rhombic triacontahedron with its shifts in various quasilattice directions ?

Response :

The decomposition of K into cells, corresponding to the 24 local environments, are precisely obtained as intersections of suitable translations of K .