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QUASIPERIODIC PATTERNS

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Résumé - Nous exposons une théorie des pavages et plus généralement des structures quasi-périodiques présentant un ordre orientationnel global. Nous présentons notre "méthode de la bande" (une variante des méthodes de projection) sur un modèle unidimensionnel. Nous exposons ensuite le cas de la symétrie icosaédrique en vue de l'application aux quasi-cristaux du type Aluminium-Manganèse. La méthode proposée donne accès aux propriétés tant locales (classification des environnements possibles de chaque site) que globales (calcul explicite de la transformée de Fourier).

Abstract - We present a theory of quasiperiodic tilings and more general quasiperiodic patterns with long range orientational order. We explain our "strip method" (a variant of the projection methods) on a one dimensional model. Then the icosahedral case is investigated in view of the quasicrystals of the type Al-Mn. Our method allows the study of the local properties (such as the classification of the vertex neighbourhoods) as well as the global ones, and an analytic expression of the Fourier transform is derived, exhibiting the quasiperiodicity.

INTRODUCTION

This lecture deals with the theory of quasiperiodic tiling, and more generally with quasiperiodic patterns. We present the ideas introduced in [9], which we call the "strip method".

The interest for non periodic tilings came first from problems of mathematical logic. However, since the invention by R. Penrose of his well known aperiodic tiling of the plane [1,7], the motivation has changed to the study of the geometrical properties of these patterns. After the first theoretical work by R. Penrose, J. Conway [7] and N.G. de Bruijn [2], A.L. Mackay [3] and Mosseri and Sadoc [4] have drawn attention to the possible implications of these structures for solid state physics. A 3-dimensional generalization of the Penrose tiling (using two rhombohedra instead of two rhombs) has been devised by R. Ammann and theoretically described by Kramer and Neri [5,6] in the context of the de Bruijn approach.

The special properties of the Fourier transform of the Penrose patterns, which are now identified as their quasiperiodicity, have been empirically observed by A.L. Mackay, using optical methods. D. Levine and P. Steinhardt have suggested in ref. [8] to take quasiperiodicity as the basis to build icosahedral quasicrystals.

The experimental discovery of icosahedral symmetry together with some kind of long range spatial order in solids by D. Schechtman, I. Blech, D. Gratias, and J.W. Cahn [10] has aroused an intense activity among theorists, as well about on the structural problem [6,8,9,11,12,13,14,15], and about stability questions which will not be

discussed here.

The theory described here, which takes into account both the icosahedral symmetry and the quasiperiodicity of the tiling, is based on an idea independently introduced in this context by V. Elser [12, 13] and us [9,15] (following N.G. de Bruijn).

A ONE DIMENSIONAL MODEL

Let us begin by a description of this method in the simplest one-dimensional case (see Fig. 1) : to tile of a straight line with two types of intervals, we start with the square lattice \mathbb{Z}^2 in the plane \mathbb{R}^2 , in which the line E to be tiled is drawn. Consider now the strip obtained by shifting the unit square K of the lattice along the line. The claim is that, 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 falling inside the strip. It just remains to project this broken line orthogonally on the given direction to get the predicted tiling, the two tiles a and b being clearly the projections of the vertical and horizontal edges of the unit square K .

One can understand the essential features of our tiling with this simple example. Consider first the choice of the unit square to build the strip. It is clear that one has to take a unit cell of the lattice in order to obtain a tiling (by the projections of the edges of the cell) : with a narrower strip, one would get "holes" in the broken line, and with a larger strip, one would get extra points. However, any unit cell of \mathbb{Z}^2 is possible, and not only the canonical square. This is closely related to the self-similarly properties of these tilings.

Secondly, consider the slope of the line E with respect to the canonical basis of \mathbb{R}^2 . It is clear that the tiling is periodic if and only if this slope is a rational number : in fact, the slope is just the ratio of the relative abundances of each type of tiles, and this ratio is certainly rational for a periodic tiling.

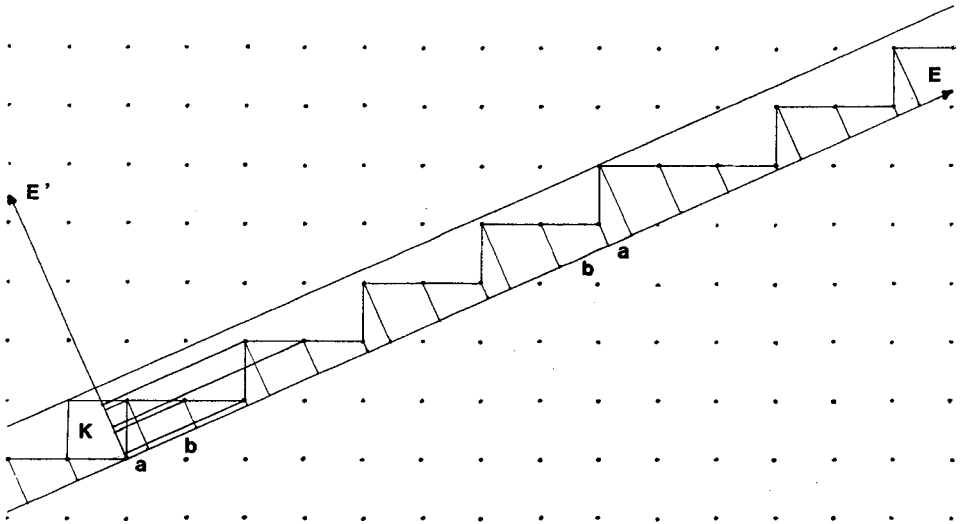


Fig. 1

The strip method in one dimension : the strip is obtained by translation of the unit square K along the line E . The unique broken line contained in the strip projects on E a tiling by means of the two tiles a and b which are the projections of the 2 edges of K .

Now, given an irrational slope, consider what happens when the strip is translated in \mathbb{R}^2 : each time a point leaves the strip, another point enters the strip. These two points are the vertices of the 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 change of the tiling, but for any finite translation of the strip (transverse to its direction) such jumps occur infinitely many times, in such a way that for each irrational slope, this construction generates a non countable set of different tilings (of course, each time the translation belongs to \mathbb{Z}^2 , one gets merely a translation of the initial tiling).

Notice that we can slightly generalize the construction and distinguish between the line along which the strip is built and the line on which the broken line is projected

to obtain the tiling. It is clear that the orientation of this last line (the tiled one) merely defines the relative sizes of the tiles, and that the orientation of the strip defines all the important properties, for instance the relative abundance of each type of tile. If we vary the orientation of the strip while maintaining unchanged the tiled line, we get different tilings with the same pair of tiles. Each time the slope is rational, the tiling is periodic, in such a way that the non periodic tiling obtained for irrational slopes can be thought of as "interpolations" between periodic lattices.

Let us now explain why any finite patch of tiles that belongs to a tiling appears infinitely many times in any tiling defined through a strip with the same given irrational slope (Conway's local isomorphism property, see [7]). Consider such a tiling, pick any finite patch of tiles in it, and consider the finite broken line that projects on this patch. Since the slope is irrational, it is clear that the projection of this broken line on E' (see fig.1) is strictly smaller than the projection of the whole strip, in such a way that there exists an open set (non empty!) of translations in E' that keep the projection of the finite broken line inside the strip. Now consider the auxiliary strip that projects on E' onto this set of translations: there are infinite vertices of \mathbb{Z}^2 inside it, and each of them defines a translation that maps the finite broken line inside our main strip onto a copy of it, which is indistinguishable from a part of the infinite broken line that projects on the tiling. This shows that any finite patch which appears in a tiling, appears infinitely many times. One can show with the same type of argument that, given any two parallel strips and a finite broken line in one of them, there always exists a translation in \mathbb{Z}^2 that maps the finite broken line inside the other strip, which means that any finite patch that appears in one tiling appears in all the tilings associated with the same slope. There are interesting questions concerning the distance between two copies of a given patch. It can be shown that the rate of "rarefaction" of the copies of a patch when its size increases depends on arithmetical properties of the slope. For algebraic numbers, the mean distance between two copies is proportional to the size of the patch, but for Liouville numbers, the mean distance can grow arbitrary quickly.

Finally, let us describe the calculus of the Fourier transform of the measure defined by putting one Dirac delta at each vertex of the tiling (fig. 2). Following the strip method, 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. To compute the Fourier transform, we have just to operate the "Fourier images" of these three steps in the reciprocal space. The first one is to take the Fourier transform of the square lattice, which is of course another square lattice of Dirac deltas. The second step is the convolution by the Fourier transform of the characteristic function of the strip, which is easy

to compute since it is a product: in the direction E^* dual to the direction of the strip, this Fourier transform is a Dirac delta and in the orthogonal direction

E'^* , it is the smooth function $(\text{sinc})/k$, up to normalizations and phase factor. To complete the convolution, we have to translate a copy of this Fourier transform at each point of the reciprocal lattice. The third step (The Fourier image of the projection) is merely the restriction to the line E'^* , as shown on fig. 2.

Let us make a few comments about the result. The most important point is that the Fourier transform thus obtained is a sum of weighted Dirac deltas, carried by the projection of the whole lattice \mathbb{Z}^2 , i.e. by a two generators \mathbb{Z} -module, and this property of the support of its Fourier transform is the very definition of the quasi periodicity of a measure. Observe that the quasiperiodicity follows directly from the strip being built on a straight line : one could produce more general tilings with a strip obtained by shifting the unit cell along a curved or undulating line (while maintaining the projection on a straight line) and they would not be quasi-periodic. The second point is that a translation of the strip changes the Fourier transform only by a phase factor (a different one for each Dirac delta) in such a way that all the tilings associated with the same irrational slope give the same diffraction patterns, as far as only intensities are measured.

Finally, observe that although the support of the Fourier transform is a dense set, the intense peaks correspond to vertices which are near the line E^* (see fig. 2), and that the set of peaks whose intensity is greater than any strictly positive threshold is always discrete. In fact, the quantitative analysis of the intensities in the diffraction pattern may be used to reconstruct the geometry in the direct space (up to a translation of the strip) in the same sense and with the same limitations as in ordinary crystallography.

THE GENERAL CASE

We give now the generalisation of this method to arbitrary dimensions. We generate a quasiperiodic tiling of a p -dimensional space E as the projection, from a higher dimensional space \mathbb{R}^n , of a p -dimensional surface made up of a suitable union of p -facets of a regular n -dimensional lattice L in \mathbb{R}^n .

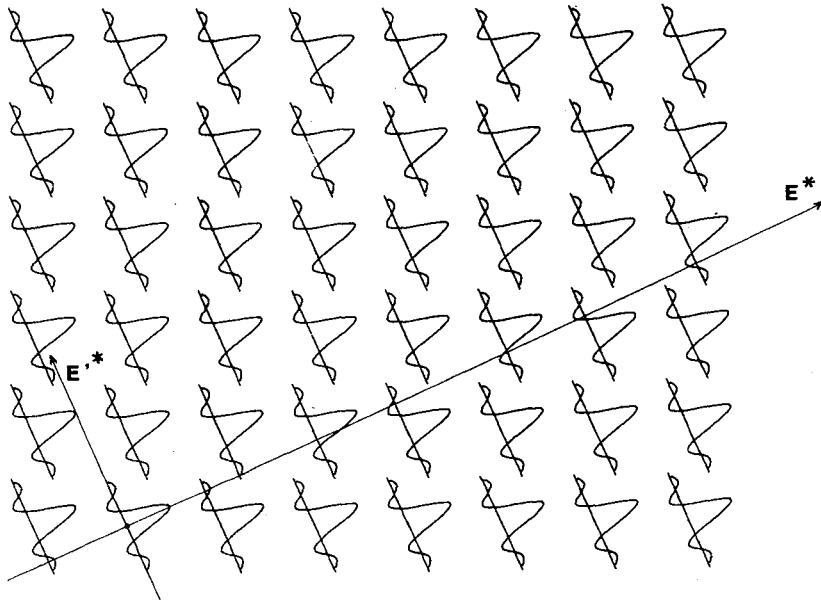


Fig. 2

Construction of the Fourier transform of the 1-dimensional tiling.

Actually, let $L = \mathbb{Z}^n$ be the n -dim lattice in \mathbb{R}^n generated by the natural basis $[e_1, \dots, e_n]$, and let γ_n be the unit cube. Let $E \subset \mathbb{R}^n$ be a p -dimensional subspace of \mathbb{R}^n , and assume that E does not contain any point of the lattice, except the origin.

There are $\binom{n}{p}$ different p -facets (the p -dimensional analog of an edge) of γ_n containing the origin. These facets project on E on a-priori $\binom{n}{p}$ different p -volumes. A tiling of E by mean of these volumes is obtained in the following way: Let $S = E + \gamma_n$ be the open strip generated by shifting γ_n along E . Then the claim is that the union of all p -facets entirely contained in S is exactly a p -dimensional surface of \mathbb{R}^n , the projection of which on E gives the announced tiling.

If E' is the orthogonal complement of E in \mathbb{R}^n , the projection K of the strip on E' is just the projection of the unit cube γ_n . Moreover, if $E \cap L = \{0\}$, the projection of the lattice L in E' is one to one. Thus the set of vertices of the quasiperiodic tiling corresponds to the set of points of L that project in E' inside K .

Now, if E is invariant under the action of a subgroup G of the point group of the lattice L , the a-priori $\binom{n}{p}$ different tiles fall into classes, in such a way that the tiles of each class have the same shape, and are permuted by G .

The set of p -volumes around a given vertex x of the tiling is completely specified by the set of corresponding p -facets falling in K around the corresponding point x' in E' . Note that no $(p+1)$, $(p+2)$, ..., n -facet of L can project in E' strictly inside K .

THE ICOSAHEDRAL CASE

Let us now specialize to the case of the icosahedral symmetry. The simplest construction involves \mathbb{R}^6 endowed with an orthogonal representation of the icosahedral group G , which permutes \mathbb{Z}^6 and such that \mathbb{R}^6 falls in two G -invariant 3-spaces, E and E' equipped with non equivalent irreducible representations of G .

The 20 different 3-facets of $L = \mathbb{Z}^6$ fall in E (and E') on different rhombohedra, with the same facets (with angles $\text{Atn}(2)$ and $\Pi - \text{Atn}(2)$), each of which being repeated 10 times. These are the rhombohedra considered by A.L. Mackay in [3], P. Kramer and R. Neri in [5,6], and us in [9] (Fig. 3b and c).

The open strip is defined by $S = E + \gamma_6$ where γ_6 is the open unit cube of \mathbb{R}^6 .

It can be seen that the projections $\Pi(L)$ on E and $\Pi'(L)$ on E' are \mathbb{Z} -modules which are dense in E and E' . If $\varepsilon_1, \dots, \varepsilon_6$, is the natural basis of \mathbb{R}^6 , $\Pi(\pm\varepsilon_1), \dots, \Pi(\pm\varepsilon_6)$ point to the 12 vertices of a regular icosahedron centered at the origin of E and so do $\Pi'(\pm\varepsilon_1), \dots, \Pi'(\pm\varepsilon_6)$ in E' .

The projection $\Pi(S \cap L)$ in E is in one to one correspondance with the other projection $\Pi'(S \cap L) = K \cap \Pi'(L)$ where $K = \Pi'(\gamma_6)$ is a rhombic triacontahedron (fig. 3a).

The fact that no (closed) 4-facet of \mathbb{Z}^6 can project inside K insures that a non-periodic tiling of E by mean of the two types of rhombohedra is obtained.

The vertex neighbourhood around a given point x in E is completely specified by the set of 3-facets around the corresponding point x' in E' . Now observe that for a given rhombohedron (spanned by (e_i, e_j, e_k)) to be entirely contained in the triacontahedron, it is necessary and sufficient that each of its vertices

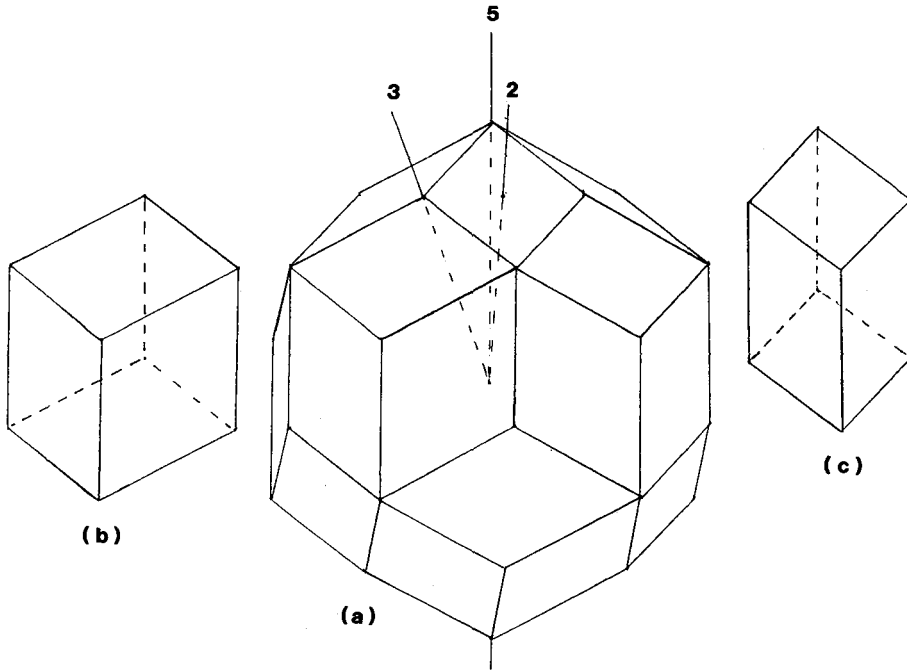


Fig. 3

The projection (a) of the unit cube of \mathbb{R}^6 in E and E' is a triacontahedron. A 5-fold axis, a 3-fold axis and 2-fold axis are represented. In (b) a flat rhombohedron and in (c) a thick rhombohedron, which are the 2 tiles of the icosahedral tilings.

fall inside an other rhombohedron, spanned by e_1, e_m, e_n , in such a way that (i,j,k,l,m,n) is a permutation of $(1,2,3,4,5,6)$, and located in the triacontahedron in one of eight canonical positions according to the vertex considered. Looking for the intersections of these 160 rhombohedra yields a cell decomposition of the triacontahedron in which each cell corresponds to a vertex neighbourhood. One thus can see that, up to the symmetry operations, there are only in these tilings 24 possible patterns of rhombohedra around a point. In particular the central cell of the triacontahedron corresponds to a 20-pronged star with the icosahedral symmetry.

We present in Fig. 4,5 and 6 three sections of this tiling, which are associated to axes of order 5, 3 and 2 respectively. The cuts, which are made along 2-dimensional surfaces taken from 2-facets of the tiling, yield quasiperiodic tilings of the plane. Actually the first section, carried out orthogonally to a 5-fold axis, projects on a generalised Penrose tiling. The two other sections project on quasiperiodic tilings of the plane associated with 3-fold and 2-fold symmetries.

As in the one dimensional case, the strip can be translated, which yields an uncountable set of non-isomorphic tilings.

One of the most striking features of all these tilings, is their quasiperiodicity, in the sense that for any tiling, the measure defined by a Dirac delta at each

vertex, is quasiperiodic : its Fourier transform is a sum of weighted Dirac measures with support in the \mathbb{Z} -module generated by the projections of the basis vectors of the lattice. Moreover, all tilings have the same Fourier transform, up to a phase at each point, in such a way that they are identical from a "diffractive" point of view.

In fact, the calculus of the Fourier transform runs exactly as in the one dimensional case. Here is a brief account of the proof : let $\nu = \chi_S \sum_{\xi \in \mathbb{Z}^6} \delta_\xi$ be the

measure associated to $S \cap \mathbb{Z}^6$, where χ_S is the characteristic function of the strip in \mathbb{R}^6 . Then $n = \sum_{\xi \in \mathbb{Z}^6} \chi_S(\xi) \delta_{\pi(\xi)}$ is the measure associated to the tiling in E .

If $\xi = (x, x')$ is the orthogonal decomposition of $\xi \in \mathbb{R}^6$ in E and E' , and if $\kappa = (k, k')$ is the corresponding decomposition in the dual space, the Fourier transform of n is given by $n^*(k) = \nu^*(k, 0)$. Now $\nu^* = \chi_S^* * \sum_{\lambda \in \mathbb{Z}^6} \delta_\lambda$, and since $\chi_S(x, x') = \chi_{TR}(x')$

where χ_{TR} is the characteristic function of the triacontahedron in E' ,

$\chi_S^*(k, k') = \delta(k) \chi_{TR}^*(k')$. Finally $n^*(k) = \sum_{\lambda \in \mathbb{Z}^6} \delta(k - \lambda) \chi_{TR}^*(-\lambda')$ where $\lambda = (1, 1')$ is the decomposition of λ in the dual space.

We give in Fig. 7;8 and 9, the computed Fourier transforms of a tiling, in the 3 planes respectively orthogonal to symmetry axes of order 5, 3 and 2. These patterns are astonishingly similar to the electron diffraction images obtained by D. Shechtman, I. Blech, D. Gratias and J.W. Cahn, reported in [10], on rapidly cooled alloys of Al and Mn.

The general framework presented here can be generalised in many ways. For instance if the condition which insures an exact tiling of the space is removed, more general quasiperiodic patterns are obtained.

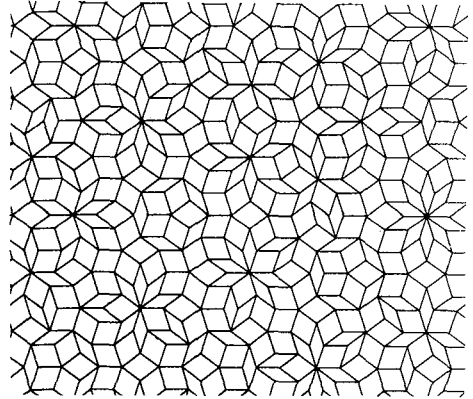
On the other hand, the projection space and the strip may have different orientations : the first one specifies the tiles while the second one dictates their relative abundance. As in the one dimension model, the quasiperiodic tiling thus obtained can be seen to interpolate between periodic ones, which correspond to rational orientations of the strip.

Notice that the quasiperiodicity of the tilings is independent of the fact that neither the pentagonal nor the icosahedral symmetries are compatible with periodic ordering. In fact the sections corresponding to the 2-fold and 3-fold axes, (given in Fig. 5 and 6), show quasiperiodic tilings of the plane while these symmetries are of crystal type.

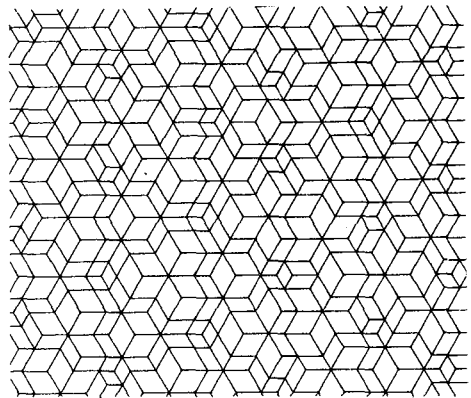
As a final remark, let us stress on the idea that the construction presented herein works in any dimension and with any lattice. For instance, it is easy to see that an other type of quasiperiodic tiling of the space with icosahedral symmetry can be obtained from \mathbb{R}^{10} , the icosahedron being replaced by a dodecahedron.

Fig. 4

A section of an icosahedral tiling, orthogonally to a 5-fold axis. A generalized Penrose tiling is obtained, with for instance a 10 pronged star.

Fig. 5

A section of an icosahedral tiling, orthogonally to a 3-fold axis.

Fig. 6

A section of an icosahedral tiling, orthogonally to a 2-fold axis.

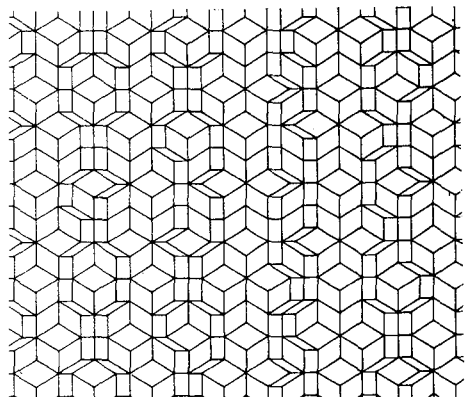
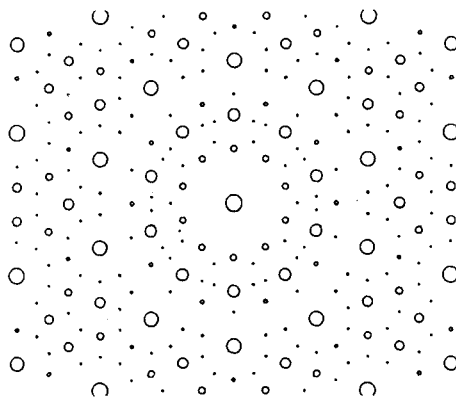
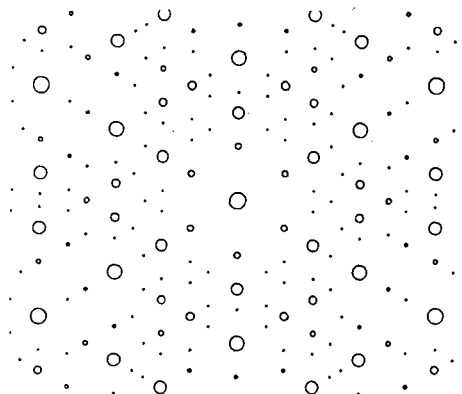


Fig. 7

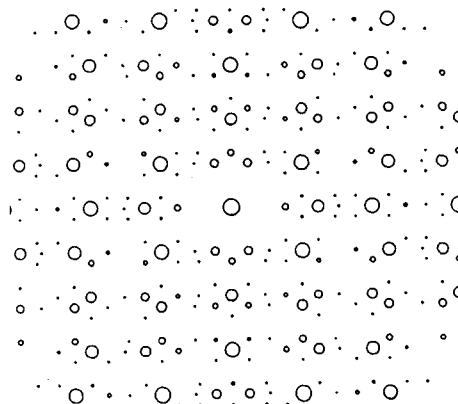
The Fourier transform orthogonal to a 5-fold axis. The peaks above a given threshold are represented by circles with radii proportional to their amplitudes.

Fig. 8

The Fourier transform orthogonal to a 3-fold axis.

Fig. 9

The Fourier transform orthogonal to a 2-fold axis.



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