

with the experimental results on phase determination from high-order multiple diffraction (Chang, Hong, Luh, Pan, Tang & Sasaki, 1988).

It should be noted that the derivation of $I_h(N)$ is a kinematical treatment. However, the use of Green functions is a dynamical approach. For example, the pole of the Green function gives the dispersion equation (Ohtsuki & Yanagawa, 1966). The real part of the equation describes the relation between the wave vectors inside the crystal and the angular deviation of the incident beam from the Bragg angle. The imaginary part of the dispersion relation defines the absorption coefficient. By solving the dispersion equation and introducing appropriate boundary conditions, the diffraction intensity $I_h(N)$ can be calculated dynamically.

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Quasiperiodic Tilings: a Generalized Grid-Projection Method

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Abstract

We generalize the grid-projection method for the construction of quasiperiodic tilings. A rather general fundamental domain of the associated higher-dimensional lattice is used for the construction of the acceptance region. The arbitrariness of the fundamental domain allows for a choice which obeys all the symmetries of the lattice, which is important for the construction of tilings with a given non-trivial

point-group symmetry in Fourier space. As an illustration, the construction of a two-dimensional quasiperiodic tiling with 12-fold orientational symmetry is described.

0. Introduction

Interest in non-periodic tilings first arose from problems in mathematical logic (Wang, 1965; Robinson, 1971). However, since Penrose's invention of his well known non-periodic tilings (Penrose, 1974, 1979; Gardner, 1977), the motivation has changed to the study of geometrical questions related to such tilings. J. Conway (see Gardner, 1977) and N. G. de Bruijn (1981) have played a dominant role in this field.

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We define a tiling as a covering of the plane by translations of a finite number of polygons with no holes or overlaps. Note, however, that, depending on the context, other definitions may be more appropriate (e.g. Grünbaum & Shepard, 1987). Here we are interested in *quasiperiodic* tilings. By this we mean:

(i) The tiling is not periodic. There exist no translations (except the identity) which leave the tiling unchanged.

(ii) If we put a δ function to each vertex of the tiling, the Fourier transform of the resulting structure is a sum of δ peaks, whose positions are integer linear combinations of a finite set of vectors $\{\mathbf{k}_1, \dots, \mathbf{k}_n\}$:

$$F(\mathbf{k}) = \sum_{\mathbf{l} \in \mathbb{Z}^n} w_{l_1, \dots, l_n} \delta\left(\mathbf{k} - \sum_{i=1}^n l_i \mathbf{k}_i\right). \quad (0.1)$$

(iii) Any finite part of the tiling appears infinitely often in the tiling.

Condition (iii) is often dropped, but the tilings we will consider have this property.

Quasiperiodic tilings may have symmetries in Fourier space which are incompatible with a periodic structure and therefore do not occur for crystals. A famous example is the Penrose tiling with fivefold symmetric Fourier transform. This has led to physicists' interest in quasiperiodic tilings, since icosahedrally symmetric diffraction patterns of an Al-Mn alloy, observed by Schechtman, Blech, Gratias & Cahn (1984), could be explained in terms of a three-dimensional version of the Penrose tiling (Mackay, 1981; Duneau & Katz, 1985; Elser, 1986; Kalugin, Kitaev & Levitov, 1986; Levine & Steinhardt, 1984). More information on the symmetry of quasiperiodic tilings and the connection with physics can be found in the Les Houches Proceedings (1986).

The main concern of this paper will be a generalization of the grid-projection method used by various authors (Duneau & Katz, 1985; Elser, 1986; Gähler & Rhyner, 1986; Kalugin, Kitaev & Levitov, 1986; Korepin, 1986; Kramer & Neri, 1984; Socolar, Steinhardt & Levine, 1985). Our algorithm projects part of an n -dimensional lattice Γ in E^n onto an irrationally embedded d -dimensional subspace. It is based on a periodic tiling of E^n by copies of a rather general fundamental domain of Γ , as opposed to Gähler & Rhyner (1986), who considered only fundamental *parallelotopes*. This extension allows for the choice of a fundamental domain whose closure obeys all the symmetries of the lattice, which is important for the construction of tilings with specified symmetry in Fourier space. The tilings so obtained are then no longer tilings by parallelotopes alone, but can contain any kind of convex polytopes. These tilings will not be the final step, however. We rather prefer to consider their Voronoi partitionings, since these seem to have more relevance to physics (Jaric, 1986; Henley, 1986).

The outline of this paper is as follows. After briefly reviewing the concepts of Voronoi partitioning and tilings by fundamental domains in §§ 1 and 2, we present our generalized algorithm in § 3. In § 4 we prove that the tilings constructed in § 3 are indeed quasiperiodic in the sense explained above. Finally, § 5 is devoted to an example to illustrate these techniques.

1. Tilings by parallelotopes and Voronoi domains

The standard grid-projection method (Gähler & Rhyner, 1986) yields tilings of the Euclidean space E^d by a finite set of parallelotopes. Possible sets of parallelotopes can be obtained as follows. Let $\{\mathbf{t}_i\}_{i=1, \dots, n}$ be a set of n vectors in E^d ($n > d$). Any subset of d linearly independent vectors of this set spans a parallelotope (see next section). With the parallelotopes obtained in this way E^d can be tiled both periodically and quasiperiodically.

It should be noted that the set of vertices of such a tiling is a special case of a Delauney (r, R) system (Delauney, 1937), which is a point set $\{v_i\}$ in E^d with the following two properties:

(i) The minimal distance between any two points of the system is $r > 0$.

(ii) Inside or on the surface of any ball of radius R , no matter where we put its centre, there is at least one point of the system.

With each (r, R) system we associate its *Voronoi partitioning* of E^d , which divides E^d into *Voronoi domains*, also called Dirichlet or Wigner-Seitz cells. The Voronoi domain associated with v_j is a convex polytope and consists of all points of E^d whose distance to v_j is not larger than the distance to any other point $v_i \neq v_j$ in the system. Note that according to this definition a Voronoi domain is a closed set, which means that boundary points belong to two or more Voronoi domains. An (r, R) system has in general infinitely many different Voronoi domains, but a quasicrystal can have only finitely many (up to shifts) (see § 3). A (periodic) lattice has only one type of Voronoi domain.

The Voronoi domain around a point v_j of an (r, R) system in E^d can be constructed as follows. Consider the set of all vertices v_i inside a closed ball of radius $2R$ centred at v_j . For each point v_i in this set, construct the $(d-1)$ -dimensional hyperplane perpendicular to the segment $v_j - v_i$ and passing through its midpoint $\frac{1}{2}v_i + \frac{1}{2}v_j$. Each of these hyperplanes cuts E^d into two half spaces. The Voronoi domain v_j is the intersection of all those half spaces which contain v_j .

2. Fundamental domains of a lattice

Consider a lattice Γ in E^n generated by n linearly independent vectors $\mathbf{e}_1, \dots, \mathbf{e}_n$. A *fundamental*

parallelopete F_p of Γ is the set

$$F_p = \sum_{i=1}^n \lambda_i \mathbf{e}_i, \quad 0 \leq \lambda_i < 1. \quad (2.1)$$

Since a lattice has infinitely many lattice bases, it has also infinitely many fundamental parallelotopes. A fundamental parallelotope is a special case of a *fundamental domain* F of a lattice, which is a measurable set with the following two properties:

(i) The translations of F by all lattice vectors of Γ cover E^n with multiplicity one.

(ii) F contains exactly one point of the lattice.

It should be noted that a fundamental domain is neither closed nor open; only a part of the boundary belongs to F . In the following we will restrict ourselves to fundamental domains whose closure is a convex polytope. Particularly interesting is a fundamental domain whose closure is the Voronoi domain. From property (ii) it follows that with each fundamental domain F a unique lattice point $\gamma(F)$ is associated. This will become important later.

3. The generalized grid-projection method

Let us decompose the space E^n containing the lattice Γ into two orthogonal subspaces, $E^n = E^\parallel \oplus E^\perp$. We will assume in the following that this decomposition is irrational, *i.e.* neither E^\parallel nor E^\perp contain any lattice vectors of Γ . Let F_0 be a fundamental domain of Γ , and $\mathcal{P}_\Gamma(F_0)$ the partitioning of E^n into all Γ translations of F_0 . The closures of the Γ translations of F_0 will be called the cells of the partitioning. We assume that the cells are convex polytopes, and that the partitioning $\mathcal{P}_\Gamma(F_0)$ is face to face, *i.e.* if two cells have a non-zero intersection, then this intersection is a (common) face of these two cells. Note that the Voronoi partitioning is always face to face. If a cell is not equal to a Voronoi domain of the lattice, we moreover assume that the partitioning is generic in the sense that a face of dimension m is contained in exactly $n - m + 1$ cells. The dual of such a partitioning is simplicial, *i.e.* all its cells (and their faces) are simplices. Next, consider a d -dimensional (affine) subspace E of E^n which is parallel to E^\parallel . We assume that E is located at a generic position, so that only faces of dimensions $n - d$ to $n - 1$ of the cells have non-zero intersection with E .

The generalized projection method is now described as follows. The vertices of the tiling are obtained by projecting orthogonally onto E the set W of lattice points whose associated fundamental domain has a non-zero intersection with E :

$$W = \{\gamma(F) \mid F \cap E \neq \emptyset, F \in \mathcal{P}_\Gamma(F_0)\}. \quad (3.1)$$

Next, we have to divide E into tiles by specifying all their faces of dimensions up to $d - 1$. The one-dimensional 'faces' are obtained by connecting all

those vertices by a straight line whose associated cells share a common face of dimension $n - 1$ which cuts E . If $d = 2$, the tiling is then completely specified. For $d > 2$, however, the situation is somewhat more complicated. Those lattice points whose associated cells share a face of dimension k are the corners of a convex polytope of dimension $n - k$. For a generic partitioning this is evident, for there are always exactly $n - k + 1$ such points. For the Voronoi partitioning, we can argue differently. The points whose cells share the k face under consideration can all be connected by a chain or net of straight lines each of which is perpendicular to an $(n - 1)$ face containing the k face and thus perpendicular to the k face itself. Therefore, all these points are contained in a single plane of dimension $n - k$ perpendicular to the k face. Hence, in both the Voronoi and the generic case we can build the $(n - k)$ -dimensional polytope dual to a given k face. If now the k face cuts E , we project its dual polytope to E . In this way we obtain a prescription for the subdivision of E into tiles. Note that with each projected dual of a k face also all its boundaries are projected, since the k face is contained in the corresponding $(k + 1)$ faces which cut E too.

The same tiling can also be obtained as the dual of a grid G . This grid is given by the intersection of the union of the boundaries of all cells of the partitioning with the subspace E . The grid divides E into convex polyhedral cells, called *meshes*, the faces of which are the intersections of E with the $(n - 1)$ -dimensional faces of the cells of the partitioning. Each mesh of the grid corresponds to a cell which cuts E . Therefore, with each mesh we can associate the projection of the corresponding lattice point, and two lattice points belonging to meshes with a common $(d - 1)$ face have to be connected by the projection of the corresponding lattice vector connecting the two lattice points. The vertices associated with the meshes sharing a common k face will become the corners of a $(d - k)$ face of a tile [these vertices are indeed contained in a $(d - k)$ plane as explained in the previous paragraph]. In this way we see that the tiling obtained previously by projection can be reconstructed from the grid. According to this construction, it is the dual graph of the grid.

What is not immediately clear is whether there will be overlapping tiles, *i.e.* whether the tiling is folded. Whether there are additional conditions required to avoid overlapping, and what these conditions would be, we leave as an open problem. For the Voronoi case, however, we have some (numerical) evidence that overlapping does not occur, and we conjecture that this is generally true for the Voronoi case. For the classical grid method, the necessary and sufficient non-overlapping conditions have been determined (Gähler & Rhyner, 1986; de Bruijn, 1986).

From the grid picture and from the periodicity of Γ it follows that the tiling consists only of a finite

number of different tiles (up to translation), for there are only finitely many inequivalent $(n-d)$ faces of the cells of the partitioning which can cut E [note that the type of such an $(n-d)$ face determines which vertices belong to the associated cell]. By a similar reasoning one finds that there are only finitely many arrangements of cells which share a common vertex, so that the Voronoi partitioning of the tiling, as constructed in § 1, consists of a finite number of different cells too. Bounds on the number of different patches of radius R of such a quasiperiodic tiling have been obtained by Gähler (1986). This number is finite and can grow only with a fixed power of R .

Let us compare our construction briefly with the algorithm proposed by Gähler & Rhyner (1986). They consider only special fundamental domains, namely parallelotopes. This has the disadvantage that for non-orthogonal lattices it is impossible to choose a parallelotope which is invariant under the whole point group of the lattice Γ . The choice of a symmetric fundamental domain is essential for the construction of quasiperiodic tilings which have the corresponding symmetry in Fourier space. By allowing a more general fundamental domain, e.g. the Voronoi domain, this deficiency is removed. This additional freedom is the main difference compared with Gähler & Rhyner (1986). The use of different 'grid' and 'tiling spaces' or inclusion of a subsequent linear transformation applied to the tiling could of course also be incorporated into the present algorithm.

4. Proof of quasiperiodicity

In this section we demonstrate that the tilings constructed in the last section satisfy the three conditions for quasiperiodicity formulated in the *Introduction*. Since the proof of condition (ii) is a standard one (e.g. Gähler & Rhyner, 1986; Zia & Dallas, 1985), we restrict ourselves to conditions (i) and (iii).

First we prove non-periodicity. Let us define the projectors P^\parallel and P^\perp projecting orthogonally onto E^\parallel and E^\perp respectively. Further, define the *strip* S as

$$S = \{\mathbf{m} + \mathbf{e} \mid \mathbf{m} \in M, \mathbf{e} \in E^\parallel\}, \quad (4.1)$$

where the *acceptance region* M is the projection $P^\perp F$ onto E^\perp , with F a translation of F_0 centred at E . Then, we can write the set W defined in (3.1) as $W = \Gamma \cap S$. Clearly, the projection of W onto E^\parallel , $W^\parallel = P^\parallel W$, is the set of vertices of the tiling. Owing to the irrationality of the embedding of E^\parallel and E^\perp , the sets $P^\parallel \Gamma$ and $P^\perp \Gamma$ are dense in E^\parallel and E^\perp , and there is a one-to-one correspondence between Γ , $P^\parallel \Gamma$, and $P^\perp \Gamma$, as well as between W , W^\parallel , and $W^\perp = P^\perp W$. Suppose that W^\parallel is periodic, i.e. W^\parallel is invariant under a translation \mathbf{g}_\parallel . Then \mathbf{g}_\parallel maps vertices to vertices and is therefore the projection of a lattice vector \mathbf{g} . Hence, W^\parallel is also the projection of the set $W + \mathbf{g}$. Since there is a one-to-one correspondence between W and W^\parallel

this means that $W = W + \mathbf{g}$. Let us project this equation onto E^\perp : $W^\perp = W^\perp + P^\perp \mathbf{g}$. Since the closure of W^\perp is compact, this means that $P^\perp \mathbf{g} = 0$ or $\mathbf{g} \in E^\parallel$, which contradicts our assumption of an irrational embedding of E^\parallel . Therefore the tiling is non-periodic.

Now we show that every finite part $W_f^\parallel \subset W^\parallel$ has infinitely many copies in W^\parallel . Denote by W_f the unique subset of W such that $W_f^\parallel = P^\parallel W_f$, and by W_f^\perp its projection onto E^\perp . Since E is at a generic position, no lattice points are projected onto the boundary of M , and so W_f^\perp is in the interior of M . Let Δ be the distance of W_f^\perp to the boundary of M ,

$$\Delta = \min_{\substack{\mathbf{x} \in W_f^\perp \\ \mathbf{y} \in \partial M}} \{|\mathbf{x} - \mathbf{y}|\}. \quad (4.2)$$

For every lattice vector \mathbf{g} whose projection onto E^\perp is inside an open ball of radius Δ , we have the result that the finite set $\tilde{W}_f = W_f + \mathbf{g} \subset \Gamma$ projects into M , $P^\perp \tilde{W}_f \subset M$, and therefore belongs to the strip S . This means that a translation by $P^\parallel \mathbf{g}$ maps W_f^\parallel onto an equivalent set. Since $P^\perp \Gamma$ is dense in E^\perp , there are infinitely many such lattice vectors, and so the proof is completed.

5. Example: a dodecagonal tiling

As an application, we discuss the construction of a class of two-dimensional tilings with 12-fold-symmetric Fourier spectrum. These tilings were first constructed by Stampfli (1986) by means of a grid. They may be relevant for the description of quasicrystalline Ni-Cr (Ishimasa, Nissen & Fukano, 1985; Gähler, 1988). More details about these and related tilings can be found in Gähler (1988).

The relevant lattice for our case is the *diisohexagonal orthogonal primitive* lattice (Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, 1978) in four dimensions, denoted by Γ . This lattice has a point-symmetry group which contains the subgroup D_{24} . The latter is the relevant symmetry group for our purposes. The lattice Γ is easily constructed as follows. Let us decompose E^4 into two orthogonal subspaces, $E^4 = E^\parallel \oplus E^\perp$. E^\parallel is the space onto which we will project. Let $\{\mathbf{e}_1, \dots, \mathbf{e}_{12}\}$ be a star of 12 vectors in E^4 such that their projections onto E^\parallel and E^\perp are given by

$$\begin{aligned} \mathbf{e}_i^\parallel &= (\cos[\pi(i-1)/6], \sin[\pi(i-1)/6]) \\ \mathbf{e}_i^\perp &= (\cos[5\pi(i-1)/6], \sin[5\pi(i-1)/6]) \end{aligned} \quad (5.1)$$

with respect to Euclidean coordinates in E^\parallel and E^\perp . The vectors $\{\mathbf{e}_5, \dots, \mathbf{e}_{12}\}$ can be expressed as integer linear combinations of the remaining four vectors, and since $\{\mathbf{e}_1, \dots, \mathbf{e}_4\}$ are rationally independent, the set $\{\mathbf{e}_1, \dots, \mathbf{e}_{12}\}$ generates a four-dimensional lattice which will be identified with Γ .

In this example, we choose a fundamental domain whose closure is the Voronoi domain. Therefore we

have to construct the Voronoi partitioning of Γ . We note that the space spanned by \mathbf{e}_1 and \mathbf{e}_3 , denoted by E^a , is orthogonal to the space E^b spanned by \mathbf{e}_2 and \mathbf{e}_4 . The vectors \mathbf{e}_1 and \mathbf{e}_3 generate a 2D regular hexagonal lattice Γ^a in E^a , and \mathbf{e}_2 and \mathbf{e}_4 generate a corresponding lattice Γ^b in E^b . Therefore, Γ is given as an orthogonal sum of two 2D regular hexagonal lattices,

$$\Gamma = \Gamma^a \oplus \Gamma^b. \quad (5.2)$$

Next we recall the fact that in such a case the Voronoi domain of Γ is given by the topological product of the two Voronoi domains of Γ^a and Γ^b ,

$$V = V^a \times V^b, \quad (5.3)$$

which of course are regular hexagons. Let H^a and H^b be the hexagon nets given by the boundaries of all Voronoi domains of Γ^a and Γ^b respectively. Then the union of the boundaries of all Voronoi domains of Γ is given by

$$N = (H^a \times E^b) \cup (E^a \times H^b), \quad (5.4)$$

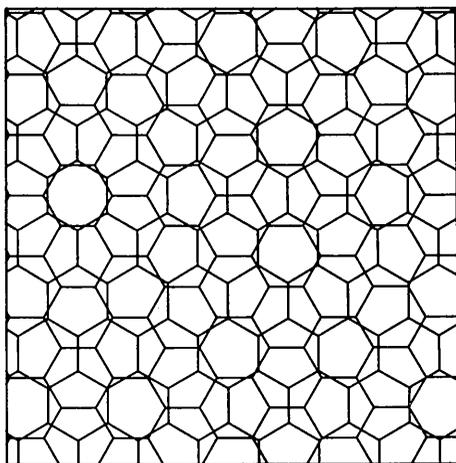


Fig. 1. Grid given by two hexagon nets.

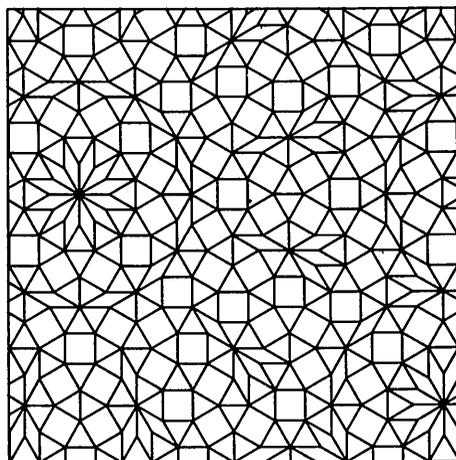


Fig. 2. Quasiperiodic tiling dual to grid of Fig. 1.

i.e. N is the union of two orthogonal arrays of hexagonal 'tubes'. Let E be a generic plane parallel to E^\parallel . The *grid*, *i.e.* the intersection of N with E , is then the union of the intersections of the two arrays of tubes, which are both regular hexagon nets, turned with respect to each other by 30° (see Fig. 1). The elementary hexagons of these nets are by a factor of two larger than the projections of the Voronoi domains of the hexagonal lattices. The relative positions of the two nets are determined by the position of E .

For the construction of Stampfli's tilings, the two algorithms discussed in § 3 now read as follows:

A. Projection construction

Project the centre of all those Voronoi domains of Γ onto E^\parallel which cut E . Connect all those points by a straight line whose Voronoi domains have a face in common which cuts E .

B. Grid construction

With each mesh of the grid $N \cap E$, associate a vertex of the tiling. If the meshes of two vertices have a common face, these vertices are connected by a line of unit length which is perpendicular to this face. This is Stampfli's prescription.

A tiling constructed in this way is shown in Fig. 2.

Let us finally note that this is a particularly simple example, owing to the fact that Γ is an orthogonal sum of two 2D lattices. From this it follows that the grid $N \cap E$ is the union of two simple periodic grids. In the general case, $N \cap E$ would be very complicated, but nevertheless all our constructions would go through as well.

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A Maximum Entropy Derivation of the Integrated Direct Methods–Isomorphous Replacement or Integrated Direct Methods–Anomalous Scattering Probability Distributions

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Abstract

It is shown that taking the appropriate terms from a series expansion of the Shannon–Jaynes entropy of a density map subject to intensity constraints gives the standard direct methods structure factor probability distribution functions. The use of two maps, one to represent a native structure, the other to represent either heavy atoms or the number density of anomalous scatterers, and the application of a similar expansion to the total entropy of both maps rapidly gives either the integrated direct methods–single isomorphous replacement or the integrated direct methods–anomalous scattering probability densities.

1. Introduction

The techniques of probabilistic direct methods have been applied to pairs of isomorphous structures (single isomorphous replacement, SIR) (Hauptman, 1982*a*; Karle, 1983, 1984*b*; Giacovazzo, Cascarano & Zeng Chao-de, 1988), and to structures containing anomalous scatterers (single-wavelength anomalous scattering, SAS) (Hauptman, 1982*b*; Giacovazzo, 1983; Karle, 1984*a, b, c*), and give rise to probability distribution functions (p.d.f.s) for combinations of the two sets of structure factors involved, *i.e.* those of the native and derivative, or of the Bijvoet pairs,

respectively. Such distributions have been obtained both for two structure factors, which are trivial in the native-only case, but now relate the native and derivative structure factors with the same index, or the two members of a Bijvoet pair, and for the six structure factors dependent on a given triplet of reciprocal space indices, from which conditional distributions of eight kinds of three-phase invariants may be found as functions of the six amplitudes. The implications of these relations have been examined in several contexts, and Karle (1986) and Fortier, Moore & Fraser (1985) give further references to these developments.

These results were obtained from the standard direct methods hypothesis of atoms randomly independently and *a priori* uniformly distributed throughout the unit cell, and follow in a similar way to the calculation of p.d.f.s of invariants for the native-only case. Extensive calculations were needed to combine the contributions of each atom towards the overall p.d.f. of the structure factors. The p.d.f. of a particular phase invariant was found by fixing the amplitudes at the measured values, and possibly also integrating out phases not involved in the invariant of interest.

Much discussion of the theory of applying maximum entropy to the phase problem has taken place in recent years (*e.g.* Collins, 1982; Wilkins,