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LETTER TO THE EDITOR

Root lattices and quasicrystals

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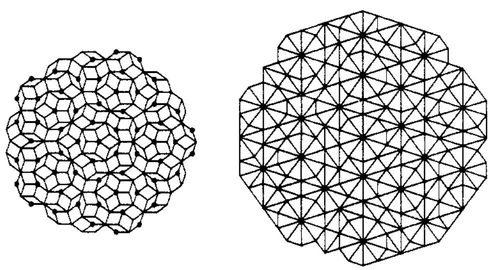
Abstract. It is shown that root lattices and their reciprocals might serve as the right pool for the construction of quasicrystalline structure models. All non-crystallographic symmetries observed so far are covered in minimal embedding with maximal symmetry.

For the construction of quasiperiodic tiling models by means of projection from higher-dimensional periodic structures, the primitive hypercubic lattices are the most frequently used ones. This has pragmatic reasons: the lattice $\mathbb{Z}^n$ is simple, exists for every positive integer n, and its symmetry (point as well as space group) is well known. Furthermore, a simple method for the generation of quasiperiodic tilings from these lattices has been established [1] which is based on a dualization scheme. However, the choice of $\mathbb{Z}^n$ is too restrictive because several patterns either require an embedding which is non-minimal with respect to the dimension of the lattice one starts from (like the Penrose pattern figure 1(a), usually derived from $\mathbb{Z}^5$ while a 4D lattice suffices, see below) or are even impossible this way (like the triangle pattern, figure 1(b)).

The question now is how to select suitable candidates from the infinite pool of higher-dimensional lattices which combine the minimal embedding of the crystallographically forbidden symmetries with a systematic and simple description. It is well known [2] that there is, up to similarity transformations, only one simple Fourier module in the plane for each non-crystallographic k-fold symmetry (up to $k = 46$) and



(a) (b)

Figure 1. Quasiperiodic patterns as obtained from the root lattice A_4, the Penrose pattern (a) with two classes of vertices and the triangle pattern (b) with two different bond lengths.

a triple of Fourier modules in 3-space with icosahedral symmetry. Therefore, from the viewpoint of general quasiperiodic densities, a single generating lattice each may be sufficient. However, from the tiling point of view, there are several inequivalent examples to be expected for each symmetry. Because a classification of tilings is not in sight, the question for a set of fundamental examples arises again.

Following this path, one is almost automatically guided to hypercubic centrings and to root lattices, or, as is immediately apparent, to root lattices and their reciprocals. Hypercubic centrings (i.e. centrings of the primitive hypercubic lattice with the full hypercubic point symmetry) give nothing new for $n=1$ and $n=2$, because they are equivalent to the primitive case. For $n=3$ one has the FCC and the BCC structure, the same being true for $n>4$ [3], where they are called F-type and I-type structures, respectively. Only $n=4$ shows a higher symmetry: F-type and I-type are equivalent and they possess a point group three times larger than the primitive lattice $\mathbb{Z}^4$. This specific 4D lattice will be of some importance in what follows.

Root lattices are those lattices which are generated by so-called root systems [4, 5], i.e. which are formed by all integer linear combinations of the vectors (roots) of those systems. These root systems form a certain class of vector stars with specific symmetries, lengths, and angles (cf [4, 6]). They occur in different contexts, e.g., in the classification of crystallographic finite reflection groups [6] or in the classification of finite-dimensional semisimple Lie algebras [5]. For the root lattices, one can derive [4] the list $A_n(n\geqslant 1)$, $\mathbb{Z}^n(n\geqslant 2)$, $D_n(n\geqslant 4)$, E_6, E_7, and E_8 of basic lattices, the orthogonal direct sums of which constitute the whole class of root lattices.

The crystallographic point group of a root lattice coincides with the automorphism group of the corresponding root system, wherefore this group is easily accessible (cf [5, 6]). The possible angles between Voronoi vectors, i.e. those vectors which actively contribute to the determination of the generalized Wigner-Seitz or Voronoi cell [4], are multiples of 60° or 90°, thus weakly generalizing the hypercubic situation (only multiples of 90°) which, of course, is contained. The Voronoi vectors of the basic lattices listed above are just the shortest elements of the generating root systems. Furthermore, all root lattices are sublattices of their reciprocals [4] (which is tantamount to the property that the scalar product between any two lattice vectors is an integer).

Let us now come to relevant examples. We will briefly stress the non-crystallographic symmetries observed so far. This selection can be regarded as an experimental input. Nevertheless, it is important to mention that applications of root lattice projections are certainly not restricted to these special cases. In 3-space, one has only the icosahedral symmetry which is both irreducibly represented and genuinely non-crystallographic. There are three different Fourier modules possible with icosahedral symmetry [2] which can, in minimal embedding, be obtained as a projection of the primitive (observed first in [7]), the F-type [8], and the I-type (no experimental evidence found up to now) hypercubic lattice in $\mathbb{R}^6$, respectively. But these three lattices are—up to normalization—just $\mathbb{Z}^6$, D_6, and D_6^R, so we are back to root lattices and their reciprocals (cf [9] and [10] for tiling models based on $\mathbb{Z}^6$ and D_6, respectively). This means that one can build tiling models for these three cases from three easily accessible lattices. Among others, the advantages are a systematic description, an analytic access to vertex and similar local statistics and a well defined Fourier theory. Furthermore, there is no other lattice with larger point symmetry which still contains a subgroup isomorphic with the full icosahedral group.

Let us now focus on 2D quasilattices with rotational symmetries of order 5, 8, 10, and 12, which occur in Nature in the form of sections through so-called T-phases

[11, 12] perpendicular to the symmetry axis. The minimal embedding requires 4D space (since $\varphi(k)=4$ for $k=5, 8, 10, 12$, where 'φ' denotes the Euler function, e.g., see [13]). The root lattices provide these embeddings with maximal symmetry, i.e. there will be no lattice of the same dimension which does the same job with a higher symmetry. The most prominent example, the Penrose pattern (figure 1(a), and its partner, the triangle pattern (figure 1(b)), are obtained from the root lattice A_4 [14]. The dimension of A_4 is four, hence it is minimal. The point symmetry that survives the projection is described by the dihedral group d_{10} and there is no 'larger' lattice in 4D space which could resolve A_4, hence A_4 yields maximal symmetry. This can be directly extracted from the classification of 4D space groups [15]. Furthermore, this covers both the fivefold and the tenfold symmetries depending on the decoration of the tiles.

An eightfold symmetry can either be realized by means of $\mathbb{Z}^4$—which gives the well known planar octagonal quasilattice [16]—or by means of D_4 [17], the only hypercubic centering in $\mathbb{R}^4$, see figure 2. This octagonal D_4 pattern is built from three triangular tiles, see figure 2, and allows a locally determined regrouping into the $\mathbb{Z}^4$ pattern which is not possible vice versa. Hence, it is natural to consider the $\mathbb{Z}^4$ pattern as a submodel of the D_4 pattern. Furthermore, the latter has the advantage that a pattern with twelvefold symmetry can also be obtained from D_4 by means of a projection in a slightly different direction, see figure 3. This dodecagonal D_4 pattern is built from four triangular tiles and seems to contain other dodecagonal patterns [13, 18] as submodels again. Additionally, one can describe a continuous transition [17] between the octagonal and the dodecagonal phase by means of a 4D rotation which is compatible with fourfold symmetry. The latter is a subsymmetry of the eightfold as well as the twelvefold pattern within the strict dualization scheme and Klotz construction [19], which all patterns

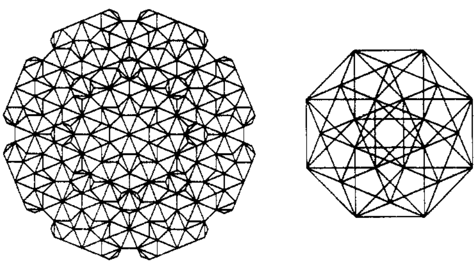


Figure 2. Quasiperiodic octagonal pattern (left) as obtained from the root lattice D_4 and projection image of the Voronoi cell of D_4 in perpendicular space.

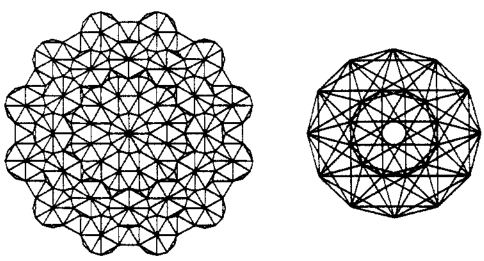


Figure 3. Quasiperiodic dodecagonal pattern (left) as obtained from the root lattice D_4 and projection image of the Voronoi cell of D_4 in perpendicular space.

shown are based on. This will provide a framework for the description of alloys like $V_{15}Ni_{10}Si$ [12] which show both symmetries in the same chemical composition.

The list of examples given above cannot imply completeness because, on the one hand, one can easily derive further patterns with a whole variety of symmetries (e.g., a heptagonal pattern may be obtained, in minimal embedding, from the 6D root lattice A_6) and, on the other hand, the relation to different other tilings [13, 18, 20], which may stem from a larger class of lattices is to be investigated in detail. This is important, because it is well known that manifestly inequivalent tilings (like the Penrose pattern and the triangle pattern) can exist which nonetheless share the same Fourier module. Currently, there is no observation of a further symmetry which is forbidden crystallographically. For the observed ones, root lattices seem to provide the right basis for structure models. Furthermore, it turns out that the minimal embedding in these experimentally realized cases always requires a description in a space with only twice the dimension of the quasiperiodic tiling. This phenomenon—if it is not accidental—should have some physical meaning while, mathematically, it is related to a certain class of deflation/inflation invariance of the quasiperiodic patterns involved. The physical aspect certainly is an interesting question for future investigations.

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