Root Lattices and Quasicrystals

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Abstract

It is shown how root lattices and their reciprocals might serve as the right pool for the construction of quasicrystalline structure models. All non-periodic 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, possible for every integer \( n \), and its symmetry (point as well as space group) is well-known. However, the choice of \( \mathbb{Z}^n \) is too restrictive because several patterns either require a non-minimal embedding (like the Penrose pattern, Fig. 1a) or are even impossible that way (like the triangle pattern, Fig. 1b). 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 that there is only one Fourier module in the plane for each noncrystallographic \( n \)-fold symmetry (up to \( n=46 \)) and a triple of Fourier modules in 3-space with icosahedral symmetry. Therefore, from the viewpoint of general quasiperiodic densities, a single generating lattice is sufficient. However, from the tiling point of view, there are several inequivalent examples per symmetry to be expected. 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 centerings and to root lattices, or, as will turn out immediately, to root lattices and their reciprocals. Hypercubic centerings (i.e., centerings of the primitive hypercubic lattice with the full hypercubic point symmetry) do not exist for \( n = 1 \) and \( n = 2 \): they give back the primitive case. For \( n = 3 \) one has the fcc and the bcc structure, the same being true for \( n > 4 \), where they are called F-type and I-type structure, respectively. Only \( n = 4 \) shows a higher symmetry: F-type and I-type are equivalent and they possess a 3-times larger holohedry than the primitive lattice \( \mathbb{Z}^4 \). This specific 4-D lattice will be of some importance in what follows.

The root lattices are those lattices which are generated by the root system of a semisimple Lie algebra (cf. [3] for details). One obtains the list \( A_n(n \geq 1), \mathbb{Z}^n(n \geq 2), D_n(n \geq 4), E_6, E_7, \) and \( E_8 \), all root lattices are constructed from by means of combinations (i.e., of direct sums). The holohedry of a root lattice coincides with the automorphism group of the corresponding root system, wherefore the symmetry is easily accessible (cf. [3]). The possible angles between Voronoi vectors are multiples of \( 60^\circ \) or \( 90^\circ \) thus weakly generalizing the hypercubic situation (only multiples of \( 90^\circ \)) which, of course, is contained.
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.

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.
Let us now come to the relevant examples. In 3-space, one has only the icosahedral symmetry which is both irreducibly represented and genuinely noncrystallographic. There are three different Fourier modules possible with icosahedral symmetry which can, in minimal embedding, be obtained as a projection of the primitive (observed first), the F-type, and the I-type hypercubic lattice in \( \mathbb{R}^6 \), respectively. But these three lattices are just \( \mathbb{Z}^6 \), \( D_6 \), and \( D_6^* \), so we are back to root lattices and their reciprocals (cf. and for tiling models based on \( \mathbb{Z}^6 \) and \( D_6^* \), respectively).

Let us now focus on 2-D quasilattices with rotational symmetries of order 5, 8, 10, and 12, which occur in nature in form of sections through so-called T-phases, perpendicular to the symmetry axis. The minimal embedding requires 4-D space (since, in each case, the Euler function is four). The root lattices provide these embeddings with maximal symmetry. The most prominent example, the Penrose pattern (Fig. 1a), and its partner, the triangle pattern (Fig. 1b), are obtained from the root lattice \( A_4 \). This covers both the fivefold and the tenfold symmetry depending on the decoration of the tiles.

An eightfold symmetry can either be realized by means of \( \mathbb{Z}^4 \) or by means of \( D_4 \), the only hypercubic centering in \( \mathbb{R}^4 \), see Fig. 2. The latter has the advantage that also a pattern with twelvefold symmetry can be obtained, see Fig. 3. Furthermore, one can describe a continuous transition between the octagonal and the dodecagonal phase within the strict dualization scheme and Klotz construction, which all patterns shown are based on. Of course, the relation to different other tilings is to be investigated in detail because manifestly inequivalent tilings (like the Penrose pattern and the triangle pattern) can exist which nonetheless share the same Fourier module.

Presently, there is no observation of a further crystallographically forbidden symmetry. For the observed ones, root lattices seem to provide the right basis for structure models, and it turns out that the minimal embedding in these cases always requires a description in a space with twice the dimension of the quasiperiodic tiling. This phenomenon - if it is not accidental - should have some physical reason and seems to be related to deflation/inflation invariance and generalized symmetries of quasiperiodic patterns. This is to be investigated in the future. Obviously, the tiling models based on root lattices should be used for structure models with realistic decorations and for the calculations of electronic and magnetic properties. Finally, quite a lot of important and interesting questions are to be answered on the way to a classification of quasiperiodic tiling models, some of which might be tackled
within the dualization scheme.

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