SYMMETRY STRUCTURE OF THE ELSER-SLOANE QUASICRYSTAL

MICHAEL BAAKE [a]
Institut für Theoretische Physik, Universität Tübingen,
Auf der Morgenstelle 14, D-72076 Tübingen, Germany

FRANZ GÄHLER [b]
Centre de Physique Théorique, Ecole Polytechnique,
F-91128 Palaiseau, France

The 4D quasicrystal of Elser and Sloane, obtained from the root lattice E_8 by the cut-and-project method, can be parametrized by the points of an 8D torus. This allows for an explicit analysis of its point and inflation symmetry structure.

1 Introduction

It is well known that the local isomorphism class (LI-class) of a crystallographic pattern $\mathcal{P}$ in $\mathbb{R}^n$ (i.e. a pattern whose periods span $\mathbb{R}^n$) consists of $\mathcal{P}$ and its translates. Since the translate $\mathcal{P}+\ell$ equals $\mathcal{P}$ for any ℓ in the lattice Λ of periods of $\mathcal{P}$, the LI-class is in one-to-one correspondence with points of a fundamental domain of Λ which (on identifying opposite facets) is an n-dimensional torus, $\mathbb{T}^n$. This can now be used to find all patterns in LI($\mathcal{P}$) with special symmetries (relative to the origin) which is a standard procedure in crystallography.

For repetitive, but non-crystallographic $\mathcal{P}$, however, the LI-class has a much richer structure and contains uncountably many ($2^{\aleph_0}$) translation classes. It is thus much more difficult to classify the complete symmetry structure of such classes, and no general answer is known. If the pattern happens to be quasi-crystallographic (in the sense that it stems from a standard projection scheme), the key to parametrizing its LI-class is to use the fundamental domain of the embedding lattice. This is the so-called *torus parametrization* that has been introduced recently [1] and then applied to some of the most frequently used quasicrystallographic tilings [1,2] in two and three dimensions.

It is the aim of this contribution to extend this set of examples to the Elser-Sloane quasicrystal in four dimensions. [3] It is constructed by the projection method from the root lattice E_8 and has the Coxeter group H_4 of order 14400 as its point symmetry group, together with an inflation/deflation symmetry with scaling factor $\tau = (1+\sqrt{5})/2$. It is of interest due to its role in the hierarchy of quasicrystals with τ inflation.

[a] Heisenberg-fellow [b] supported by the Swiss BBW (HCM programme)

2 Setup and application to inversion symmetry

In what follows, we shall use the notation and the main results of Ref. 1 without further reference. We standardize our parametrization such that the origin of the embedding space is at a lattice point of E_8, and the window (having point symmetry H_4) is symmetric around the origin of internal space. With this convention, the tiling obtained by cut-and-project with the physical space cutting through the origin has parameter $\boldsymbol{t} = \mathbf{0}$.

To each symmetry operation on the LI-class now corresponds a linear (or, more generally, affine) operator on the torus, and tilings with special properties can be found as fixed points of that operator on the torus. Also, the number of solutions can be counted: an equation of the form

$$A\boldsymbol{x} + \boldsymbol{t} \;=\; \boldsymbol{x} \mod \mathbb{T}^8 \tag{1}$$

has precisely $|\det(A - \mathbb{1})|$ different solutions, provided 1 is not an eigenvalue of A (for details, also on the singular case, see the appendix of Ref. 1).

Let us illustrate this with the simplest case, that of inversion symmetry. In view of our standardization, the corresponding operator in 8-space is defined by the isometry $\boldsymbol{x} \mapsto -\boldsymbol{x}$. Restricting this to the torus, we are thus asking for the number of solutions of $\boldsymbol{t} = -\boldsymbol{t} \mod \mathbb{T}^8$, which is $|\det(-2 \cdot \mathbb{1})| = 2^8 = 256$. They are the 2-division points of the torus (solving $2\boldsymbol{t} = \mathbf{0}$ on it). We shall see a little later how these points (and hence the tilings parametrized by them) are distributed over other properties.

There is one subtlety which has been suppressed so far: the parametrization is one-to-one only for regular members of the LI-class (those where the cut space never hits the boundary of the window), while it is multiple-to-one for the remaining singular tilings, which are then grouped into classes. [1]

3 Inflation structure

One of the most interesting properties of non-periodic tilings is the existence of inflation/deflation symmetries, and in the present case there is one with inflation multiplier τ (the golden ratio). To describe this, we start with the corresponding situation for the Fibonacci chain, discussed in detail in Ref. 1. It is shown there that one has a_n Fibonacci chains invariant under n-fold inflation, where

$$a_n \;=\; a_{n-1} + a_{n-2} + 1 - (-1)^n \tag{2}$$

with initial values $a_1 = a_2 = 1$. This follows from the determinant argument discussed above and can directly be calculated from the eigenvalues τ and $-1/\tau$ of the corresponding operator on the torus ($\mathbb{T}^2$ in this case).

This result can directly be used for our present task. The number of points on the 8-torus that are invariant under n-fold inflation (denoted by I^n) is given by the fourth power of the number a_n, because we get the same eigenvalues as before, but now with multiplicity 4. Next, let us denote by $b_n^{(4)}$ the number of fixed points under I^n which are not fixed by I^m for any $m < n$. It can recursively be calculated by

$$b_n^{(4)} \;=\; a_n^4 \;-\; \sum_{m\,|\,n,m<n} b_m^{(4)} \,. \tag{3}$$

These numbers correspond to points that can be grouped into n-cycles, so $c_n^{(4)} = b_n^{(4)}/n$ must be an integer. Table 1 lists these numbers for $1 \le n \le 8$.

n	1	2	3	4	5	6	7	8
a_n^4	1	1	256	625	14641	65536	707281	4100625
$b_n^{(4)}$	1	0	255	624	14640	65280	707280	4100000
$c_n^{(4)}$	1	0	85	156	2928	10880	101040	512500

Table 1: Inflation orbit counts of the Elser-Sloane tiling. They also apply to any other 4D cut-and-project patterns with τ-inflation.

To summarize these findings, one can attach a dynamical ζ-function to the inflation operator I on the torus. It reads

$$Z_4(x) \;=\; \frac{(1-4x-x^2)^4(1+4x-x^2)^4(1-x-x^2)^{28}(1+x-x^2)^{28}}{(1-7x+x^2)(1-3x+x^2)^{12}(1+3x+x^2)^{16}(1+x)^{32}(1-x)^{38}} \,. \tag{4}$$

This serves as generating function for the counts a_n^4 via

$$\log(Z_4(x)) \;=\; \sum_{n=1}^{\infty} a_n^4 \cdot \frac{x^n}{n} \tag{5}$$

and – through an Euler product decomposition – also for the counts $c_n^{(4)}$:

$$\frac{1}{Z_4(x)} \;=\; \prod_{n=1}^{\infty} (1-x^n)^{c_n^{(4)}} \;=\; (1-x)^1(1-x^2)^0(1-x^3)^{85}(1-x^4)^{156}\ldots \tag{6}$$

This ζ-function has the functional equation $Z_4(x) = Z_4(1/x)$ and conforms to the "Riemann hypothesis" that its zeros α satisfy $N_2[\alpha] = -1$ where N_2, the norm of the quadratic field $\mathbb{Q}(\tau)$, is defined by $N_2[r+s\tau] = r^2 + rs - s^2$.

Let us point out here that the 256 inversion symmetric tilings of section 2 coincide with the 256 tilings invariant under I^3. This is so because $\tau^3 = 2\tau + 1$ and the corresponding equations on the torus define the same set of solutions.

4 Space group and point group structure

So far, except inversion symmetry, we have only discussed inflation symmetry, which does not depend on point group symmetry. But the window of our quasicrystal is a special polytope [3] with H_4 symmetry, and so the generalized point group of the LI-class is H_4, and its space group is the semi-direct product of H_4 with the limit translation module of the tiling. The action of this space group can easily be lifted to an affine action on the torus $\mathbb{T}^8$. Since the space group is symmorphic, its action on the torus, where one computes modulo

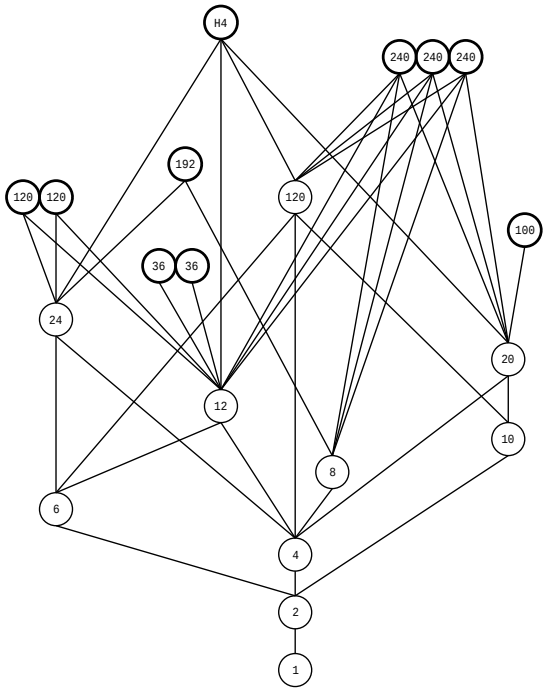

Figure 1: Classification of torus points according to their space group symmetry. Each vertex corresponds to a Wyckoff position, i.e., a class of points whose stabilizers are conjugate subgroups of the space group of the 8D periodic structure. The order of the stabilizer is inscribed into each vertex (except for H_4). Incidence relations of Wyckoff positions are indicated by connecting lines (those with smaller stabilizers contain others with bigger stabilizers). A Wyckoff position consists of a space group orbit of some (rational) affine subspace, wrapped on the torus. Vertices for Wyckoff positions of dimension zero (special points) are drawn with thick lines. They are discretely embedded on the torus. Each space group orbit of special points corresponds to one circle. Circles which touch each other represent orbits of special points with the same point group symmetry.

lattice or module translations, in fact agrees with that of the point group, so that we need not distinguish between space group and point group action.

Let us now see how single members of the LI-class reflect this point group structure, seen through their torus parameters. To this end, we have computed the set of Wyckoff positions and their incidence relations for our quasicrystal (see Fig. 1 and its caption). This was done with a program called CrystGap.[4,5] On the torus, Wyckoff positions consist of unions of subtori of various dimensions, whose points have conjugate stabilizers. Fig. 1 shows the hierarchy of these subtori (which is closely related to the classification of lower-dimensional examples[1]), together with their incidence relations. The latter also imply subgroup relations for their stabilizers, which make up an only small but essential part of the (very complex) subgroup lattice of H_4. The point groups contained in Fig. 1 as stabilizer of some point on the torus (and thus of some tiling) make up only a small fraction of the set of all subgroups of H_4.

Some points with non-trivial point group symmetry also have non-trivial inflation symmetry. Here, we shall discuss the inflation symmetry only for the special points, which are discrete on the torus. They all have a unique inflation symmetry. The only point with H_4 symmetry coincides with that of τ inflation (I) symmetry. Points in the three orbits of length 60 (stabilizer size: 240), as well as points in the orbit of length 75 (192), have I^3 symmetry. In fact, the points in these orbits make up all 255 such points. The three orbits of length 60 are permuted by I, whereas the 75-orbit is reshuffled internally by I. The two orbits of length 120 (120) and the orbit of length 144 (100) are I^4 symmetric. The pair of 120-orbits is permuted by I^2. Finally, the pair of orbits of length 400 (36) is permuted by I^4; all of its points are invariant under I^8.

Conversely to the case of I^3 symmetry, the special points do not make up all points with I^8 or even I^4 symmetry. The lacking points are to be found on the other tori, which have positive dimension. These contain, in fact, a dense set of points (all rational points) with some inflation symmetry, although of varying degree. For this reason we have confined ourselves to special points.

References

1. M. Baake, J. Hermisson and P. A. B. Pleasants, "The torus parametrization of quasiperiodic LI-classes", *J. Phys.* **A 30** (1997) 3029–56.
2. J. Hermisson, C. Richard and M. Baake, "A guide to the symmetry structure of quasiperiodic tiling classes", *J. Phys. France* **7** (1997) 1003–18.
3. V. Elser and N. J. A. Sloane, "A highly symmetric four-dimensional quasicrystal", *J. Phys.* **A 20** (1987) 6161–8.
4. B. Eick, F. Gähler and W. Nickel, "Computing Wyckoff positions and maximal subgroups of space groups", *Acta Cryst.* **A 53** (1997) 467–74.
5. F. Gähler, "Computing with crystallographic groups", this volume.