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Group Cohomology and Quasicrystals I: Classification of Two-Dimensional Space Groups

BENJI N. FISHER [a] AND DAVID A. RABSON [b]
[a] Mathematics Department, Boston College, Chestnut Hill, MA, USA
[b] Physics Department, University of South Florida, Tampa, FL, USA

Abstract

In Fourier-space crystallography, the space group is defined in terms of the point group G, the inverse lattice (or Fourier module) L, and a phase function Φ. We classify the two-dimensional space groups (or plane groups), the major step being the classification of lattices, of all ranks, symmetric under the finite point group G. This step requires new ideas from integer representation theory. Given this classification, the remaining steps can be done easily using techniques of group cohomology.

1. Introduction

Let $\rho(x)$ describe a density (such as the electron or mass density) associated to a quasicrystal. (We use the term *quasicrystal* to include all crystals, periodic or not, satisfying the conditions that follow.) A fundamental assumption of the Fourier-space description of quasicrystal symmetries [1–2] is that the density function is represented by a Fourier series of the form

$$\rho(x) = \sum_{k \in L} \hat{\rho}(x)\, e^{2\pi i k \cdot x}, \tag{1}$$

where L is a *lattice*: a finitely generated, additive subgroup of Fourier space. In the periodic case, L is a discrete subset of Fourier space; in the aperiodic case, L is not discrete, and some authors [3] prefer the term *quasilattice*. These data are enough to define the point group and space group associated to the quasicrystal. [2,4] For this note, it is enough to know that the point group G is a group of rotations g satisfying $L \cdot g = L$. (The convention used here is that vectors in real space are columns, wave vectors in Fourier space are rows, and rotations are matrices. If k is a wave vector in L and g is a rotation in G, then kg is defined by the usual rules of matrix multiplication.) Assume that G is a finite group.

Let L be a lattice symmetric under the finite point group G. Since L is a finitely generated, torsion-free $\mathbb{Z}$-module, the structure theory of modules over a principal ideal domain shows that L has a basis, say $k_1, k_2, \ldots, k_D$. That is, each $k \in L$ has a unique expression $k = n_1 k_1 + \cdots + n_D k_D$, with integer coefficients n_j. The number D is called the $\mathbb{Z}$-rank of L, analogous to the dimension of a vector space. Traditionally, one considers all lattices L, classified first by their ranks. For each lattice, one considers the group G_L of all rotations that preserve L; this group may contain

rotations of infinite order.[3] Then one considers all finite subgroups G of G_L. We call this the "L-first" approach, and advocate instead the "G-first" approach. That is, first list all finite groups of rotations; for each such group G, consider the lattices symmetric under G, or *G-lattices*. The G-lattices L_1 and L_2 are equivalent if the pairs (G, L_1) and (G, L_2) are in the same arithmetic crystal class[4] (but without the restriction on G_{L_1} and G_{L_2}).

In two and three dimensions, the list of finite subgroups of the orthogonal group is well known, and this paper describes the classification of G-lattices when G is a finite group of rotations in the plane. We are not aware of any comparable results using the L-first strategy. Many authors[2,5–6] assume that the lattice has minimal rank consistent with its symmetry. The main contribution of this paper is to remove this assumption.

In two dimensions, the point group is either $C_N = \langle r \rangle$ (cyclic of order N) or $D_N = \langle r, m \rangle$ (dihedral of order $2N$). Mermin *et. al.*[5] interpreted C_N-lattices (or N-lattices in their terminology) in terms of algebraic number theory. This leads to the observation that, even when restricting to G-lattices of minimal rank, there are many inequivalent lattices when N is large. The methods described here build on this interpretation, but for reasons of space and simplicity of exposition we will pretend that there is only one C_N-lattice of minimal rank. Thus the statements made here are strictly true only for $N < 23$ (or even numbers $N < 46$).

If the two-dimensional Fourier space is identified with the complex plane, so that the rotation r corresponds to multiplication by ζ, then a C_N-lattice is the same thing[5] as a torsion-free module over the ring of cyclotomic integers

$$R = \mathbb{Z}[\zeta], \qquad \zeta = e^{2\pi i/N}. \tag{2}$$

For small values of N, the ring R is a principal ideal domain. For large N, it is a Dedekind domain (the next best thing). The structure of modules over Dedekind domains is given by Steinitz's Theorem.[7] If Fourier space is identified with the complex plane in such a way that the mirror reflection m corresponds to complex conjugation, then a lattice symmetric under the dihedral group $G = D_N = \langle r, m \rangle$ is a module over the *twisted group ring*

$$\Lambda = \mathbb{Z}[\zeta, \sigma], \qquad \zeta = e^{2\pi i/N}, \quad \sigma^2 = 1, \quad \sigma\zeta = \zeta^* \sigma, \tag{3}$$

This is a non-commutative ring, except when $N \leq 2$. The structure of D_N-lattices is deduced from the representation theory[8–9] of the ring Λ.

2. Cyclic Point Groups

Consider the lattice L symmetric under the cyclic group $G = C_N = \langle r \rangle$. Since L is a finitely generated, torsion-free module over R, it follows that L has an R-basis $k_1, k_2, \ldots, k_d$. That is, each $k \in L$ has a unique expression

$k = a_1 k_1 + \cdots + a_d k_d$, with coefficients a_j in R. The $\mathbb{Z}$-rank D is related to d, the *R-rank* of L, by $D = \phi(N) \cdot d$. (Here, $\phi(N)$ denotes Euler's totient function, the $\mathbb{Z}$-rank of R.) In particular, the $\mathbb{Z}$-rank of L is always a multiple of the minimal rank $\phi(N)$.

Another way of stating this result is that L decomposes into the G-sublattices $L_j = Rk_j$. Multiplication by k_j amounts to rescaling and rotating by fixed amounts. Thus each L_j is geometrically similar to the standard G-lattice R. Thus there is only one G-lattice of minimal rank (up to equivalence) and a G-lattice of higher rank decomposes into copies of this fundamental lattice. This decomposition reduces the problem of calculating phase functions on L to the special case $L = R$.

3. Dihedral Point Groups

Now let L be a lattice symmetric under the dihedral group $G = D_N = \langle r, m \rangle$. It is convenient to assume that N is even. Since L is symmetric under the inversion, nothing is lost: if N is odd, then any D_N-lattice is also a D_{2N}-lattice, and *vice-versa*; the algebraic version of this observation is that $R_N = R_{2N}$ when N is odd. There are three cases to consider.

First, suppose that $N/2$ is not a prime power: $N = 12, 20, \ldots$. As in the cyclic case, the G-lattice L has an R-basis $k_1, k_2, \ldots, k_d$. Furthermore, one can choose this basis so that each k_j lies on the real axis (mirror line of m). Thus each C_N-sublattice $L_j = Rk_j$ is also a D_N-sublattice, and again the lattice L decomposes into these sublattices. In other words, a G-lattice of arbitrary rank decomposes into G-sublattices of minimal rank, each equivalent (by a rescaling, no rotation) to the standard G-lattice R.

Second, suppose that $N/2$ is an odd prime power: $N = 6, 10, 14, 18, \ldots$. Again there is an R-basis, but now there are two possibilities for each basis vector: either k_j lies on the real axis, so $k_j m = k_j$, or else it lies on the line through $1 + \zeta^*$, so $k_j m = \zeta k_j$. In other words, a G-lattice of arbitrary rank again decomposes into G-sublattices of minimal rank, but now there are two inequivalent such lattices: the standard G-lattice R, and the standard lattice rotated through the angle π/N.

Consider the example $N = 6$. The standard lattice is the familiar discrete hexagonal lattice, with one of the shortest vectors (and its negative) along the x-axis. The second lattice is also hexagonal, but with the x-axis going between shortest vectors. In the L-first approach to classification, these lattices are identified and a distinction is made between two different "settings" of the point group. Taking the G-first approach, we see one group and two lattices instead of one lattice and two groups.

Third, suppose that N is a power of 2: $N = 2, 4, 8, 16, \ldots$. In this case, there are the same two lattices of minimal rank as in the previous case and there is a third fundamental lattice to be described shortly. Consider first the distinction between the two lattices so far. To illustrate the ideas, let $N = 4$: the two lattices are the standard square lattice, with shortest

vectors along the x- and y-axes, and the square lattice with shortest vectors along the lines $y = \pm x$. In the L-first approach, these two lattices are equivalent. The only reason they are distinct in the G-first approach is that we arbitrarily choose one of the mirrors in G to identify with complex conjugation. This seems odd at first, but this distinction is necessary when describing lattices of higher rank in terms of these fundamental ones. To see this, consider an even simpler case, $N = 2$. Now, we are considering the rank-one lattices $\mathbb{Z}$ (horizontal) and $\mathbb{Z}i$ (vertical). The sum of two incommensurate horizontal lattices, or two vertical lattices, will be a one-dimensional, non-discrete lattice of rank two. The sum of a horizontal lattice and a vertical one is different: a discrete, rectangular lattice.

When $N = 2$, there are two rectangular G-lattices: primitive and face-centered. The first decomposes into two G-sublattices of rank one, as just described, but not so the second. Let a (horizontal) and b (vertical) generate a primitive rectangular lattice, and let $k = (a+b)/2$ be the vector describing the center of one of the faces. Then the face-centered lattice is generated by k and $k^* = (a-b)/2$; it contains, but does not decompose into, the rank-one lattices $\mathbb{Z}a$ and $\mathbb{Z}b$. This is typical: whenever N is a power of two, the third fundamental lattice has rank $2\phi(N)$, with an R-basis consisting of k and k^*. This lattice does not decompose into G-sublattices, and any G-lattice of higher rank decomposes into G-sublattices, each equivalent to one of the three fundamental ones.

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