Beware of 46-Fold Symmetry: The Classification of Two-Dimensional Quasicrystallographic Lattices

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The problem of classifying two-dimensional lattices with N-fold rotational symmetry for arbitrary (noncrystallographic) even N is shown to be equivalent to a much-studied problem in algebraic number theory. When translated into crystallographic language, the number-theoretic results establish that except for 29 even numbers N there are two or more distinct lattices. The smallest N for which there is more than a single lattice, however, is $N=46$. We list every N for which there is a unique lattice, and give the numbers of distinct lattices for all $N<100$.

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To describe the recently discovered quasicrystalline icosahedral[1] and decagonal[2] phases of aluminum alloys it is necessary to reexamine and extend some of the most fundamental concepts of crystallography. In particular, the most fundamental concept of all, the Bravais lattice, which can be defined very economically[3] as a discrete set of vectors closed under addition and subtraction, can be extended to the quasicrystalline case simply by deletion of the word "discrete." Only if one insists upon a minimum distance between lattice points can one restrict the rotational symmetries of Bravais lattices to twofold, threefold, fourfold, or sixfold axes.

Real-space lattices without a minimum distance between lattice points cannot describe physical structures, which are necessarily characterized by a minimum interatomic separation. Reciprocal-space Bravais lattices in this generalized sense, however, remain pertinent to the description of quasicrystalline diffraction patterns, which are indeed characterized by sets of points dense in k space.

If the classification of quasicrystals is approached through their diffraction patterns, then a crucial first step is the classification of generalized Bravais lattices. Preliminary to this, in turn, is an understanding of the possible two-dimensional generalized Bravais lattices with N-fold rotational symmetry. We address here the classification problem for such structures, making the cautionary point that the "obvious" and simplest answer is in general incorrect, although it is correct in all cases that currently seem likely to be of physical interest.

We are interested in classifying structures of the following form: Let $\mathbf{w}$ be a vector in the plane, let R be a rotation about the origin through $2\pi/N$ ($N\geq 3$) and let $\mathbf{w}^{(m)}=R^m\mathbf{w}$. By a two-dimensional generalized Bravais lattice with N-fold symmetry, which we shall call for short an "*N-lattice*," we mean a set $\mathbf{S}_N$ of vectors with the following properties: (1) Sums and differences of vectors in $\mathbf{S}_N$ are also in $\mathbf{S}_N$. (2) $\mathbf{S}_N$ is invariant under a rotation through $2\pi/N$: If $\mathbf{v}$ is in $\mathbf{S}_N$, then so is $R\mathbf{v}$. (3) Every vector $\mathbf{v}$ in $\mathbf{S}_N$ can be expressed in the form

$$\mathbf{v}=\sum_{m=1}^{N} n_m\mathbf{w}^{(m)}, \tag{1}$$

with integral n_m.

Without Property 3 there would be infinitely many distinct N-lattices even in the crystallographic cases $N=4$ or 6. The requirement 3 is equivalent to stipulating that the lattice should be integrally spanned [in the sense of (1)] by the minimal number[4] of vectors consistent with the N-fold rotational symmetry—i.e., that the N-lattices are the simplest possible structures with Properties 1 and 2.

Property 1 requires that if $\mathbf{w}$ is in $\mathbf{S}_N$, so is $-\mathbf{w}$. Since $-\mathbf{w}$ is the rotation of $\mathbf{w}$ through π, it follows that the rotational symmetry of an N-lattice is always of *even* order, and so it suffices to restrict N to even integers ≥ 4.

Two N-lattices are *equivalent* if they differ only by a scale factor and/or rotation; two N-lattices are *distinct* if they are not equivalent. Evidently the set of N-lattices can be partitioned into classes of mutually equivalent ones, such that members of different classes are distinct.

One simple N-lattice is the set $\mathbf{Z}_N$ of vectors $\mathbf{v}$ of the form (1) for *all* integral n_m, which we shall call the *standard lattice.* When N has the crystallographically allowed values 4 or 6, it is easy to show that there is just one class: All N-lattices are equivalent to the standard lattice $\mathbf{Z}_N$ (which is just the square net for $N=4$ and the triangular net for $N=6$). In the crystallographically forbidden case of major interest in the description of the quasicrystalline aluminum alloys, a rather lengthy argument[5] establishes that all 10-lattices are equivalent to $\mathbf{Z}_{10}$.

The question naturally arises whether this simple state of affairs might persist for general N. Our argument that there are no nonstandard lattices for $N=10$ sheds no light on this conjecture, exploiting detailed numerical properties of $\cos(2\pi/5)$. We shall answer the question by mapping it onto a problem that has been subject to intense scrutiny by the mathematicians.

To answer to whether a general N-lattice is equivalent to $\mathbf{Z}_N$ for arbitrary N is this: *Overwhelmingly no; but for all practical purposes, yes.* There are only 29 even values of N for which there is a single class of N-lattices; but among these are all values of N up to including $N=44$.

Thus, for example, possible structures with dodecagonal symmetry[6] can be systematically analyzed in Fourier space starting with the simple set of wave vectors (1) for *all* integral n_m. It seems improbable that quasicrystals will turn up with $N \geq 46$, but quasicrystals of any kind seemed more than unlikely just a few years ago, and so we give the complete list of the 29 N for which there is just one type of N-lattice[7]:

$$N=4,6,8,\ldots,44;\ 48,50,54,60,66,70,84,\text{ and }90. \quad (2)$$

The only cases in which there are just two classes of N-lattices are $N=56$ and $N=78$.[8] There are just three classes only for $N=46$, 52, and 72.[9] When there is not a unique N-lattice, things can be rather bizarre. The number of classes (called the *class number*, h_N) for the remaining even N below 100 are[10]

$$\begin{aligned} &h_{58}=9,\ h_{62}=9,\ h_{64}=17,\ h_{68}=32,\\ &h_{74}=37,\ h_{76}=19,\ h_{80}=5,\ h_{82}=121,\\ &h_{86}=211,\ h_{88}=55,\ h_{92}=201,\ h_{94}=695,\\ &h_{96}=32,\ h_{98}=43. \end{aligned} \quad (3)$$

In general the situation is quite horrendous. Although the number is finite for any N,[11] even for as "reasonable" a number as 128, there are 359057 distinct N-lattices. There are more than a hundred million distinct 158-lattices, more than ten billion distinct 178-lattices, and h_N grows astronomically as N gets still higher.

We have extracted these results from the mathematics literature by noticing that the problem of classifying the two-dimensional N-lattices is equivalent to a long-standing problem in algebraic number theory, the solution of which (note the dates of Refs. 8 and 9) is still not completely at hand. The tacit assumption that there is only one class of N-lattices for general N was the only fallacy in a sensational "proof" of Fermat's last theorem, announced by Lamé and avidly pursued by Cauchy in 1847. It was Kummer who discovered the multiplicity of 46-lattices, dashing cold water on these hopes.[12]

The link between N-lattices and algebraic number theory emerges when the two-dimensional vectors are viewed as complex numbers. In the complex plane we can take the N vectors $\mathbf{w}^{(m)}$ to be the Nth roots of unity:

$$\mathbf{w}^{(m)}=\zeta^m,\quad \zeta=e^{2\pi i/N},\quad m=1,2,\ldots,N. \quad (4)$$

The set of all rational linear combinations of these N roots is called the *cyclotomic field* Q_N, and the set of all integral linear combinations—i.e., our standard lattice $\mathbf{Z}_N$—is called the integers of the cyclotomic field. We shall call such "integers" *ζ-integers*, to distinguish them from ordinary integers.[13]

Consider now some subset $\mathbf{S}_N$ of $\mathbf{Z}_N$ that is also an N-lattice. Since it must be invariant under rotations through $2\pi/N$, it is invariant under multiplication of each of its elements by ζ or arbitrary powers of ζ: $\mathbf{S}_N=\zeta^m\mathbf{S}_N$. Since $\mathbf{S}_N$ is, in addition, closed under sums and differences, the product of any number in $\mathbf{S}_N$ with any arbitrary integral linear combination of powers of ζ—i.e., with an arbitrary ζ-integer—will also be in $\mathbf{S}_N$.

Such a subset of $\mathbf{Z}_N$ (closed under sums and differences and containing the product of any of its members with arbitrary members of $\mathbf{Z}_N$) is called an *ideal. The N-lattices are just the ideal of* $\mathbf{Z}_N$.

Evidently if α is any ζ-integer, the set $\alpha\mathbf{Z}_N$ given by multiplying every member of $\mathbf{Z}_N$ by α is an ideal. Such ideals, which are simply rescaled (by the modulus of α) and rotated (by the phase of α) versions of $\mathbf{Z}_N$ itself, are called *principal ideals.* Thus *every N-lattice being equivalent to* $\mathbf{Z}_N$ *is the same as every ideal of* $\mathbf{Z}_N$ *being a principal ideal.* The values of N quoted in (2) for which there is a single N-lattice are just those for which $\mathbf{Z}_N$ has only principal ideals.

More generally, when considered as sets of complex numbers two N-lattices $\mathbf{S}_N^{(1)}$ and $\mathbf{S}_N^{(2)}$ will be equivalent if there is a complex number z such that

$$\mathbf{S}_N^{(2)}=z\mathbf{S}_N^{(1)}. \quad (5)$$

In particular, if the ζ-integer α is in $\mathbf{S}_N^{(1)}$, then $z\alpha=\beta$ must be a ζ-integer in $\mathbf{S}_N^{(2)}$. Scaling both sides of (5) by α, we then have

$$\alpha\mathbf{S}_N^{(2)}=\alpha z\mathbf{S}_N^{(1)}=\beta\mathbf{S}_N^{(1)}, \quad (6)$$

where α and β are both ζ-integers.

Ideals related by (6) are called *equivalent* ideals.[14] Thus *the number of distinct classes of reciprocal lattices with N-fold symmetry is the number of distinct classes of equivalent ideals in* $\mathbf{Z}_N$. *This number,* h_N, *is called the class number* of the cyclotomic field $\mathbf{Q}_N$, and has been and continues to be the object of much computational effort.

Mathematical interest seems more focused on computing the class numbers than explicitly constructing nonprincipal ideals when $h>1$, but we have extracted from the literature the historically important specimen that established that $N=46$ is the first nontrivial case. Washington[15] shows that when $\beta=\frac{1}{2}(1+\sqrt{-23})$ the set of all ζ-integral linear combinations of 2 and β (i.e., the direct sum of $2\mathbf{Z}_{46}$ and $\beta\mathbf{Z}_{46}$) is a nonprincipal ideal, and therefore cannot be equivalent to $\mathbf{Z}_N$. To extract from this a description of a nonstandard 46-lattice it is necessary to express β as an integral linear combination of powers of $\zeta = e^{2\pi i/46}$. We have

$$-\beta = \zeta^{10} + \zeta^{14} + \zeta^{20} + \zeta^{22} + \zeta^{28} + \zeta^{30} + \zeta^{34} + \zeta^{38} + \zeta^{40} + \zeta^{42} + \zeta^{44}, \tag{7}$$

which can easily be checked numerically, or given an elementary analytical proof[16] (which, however, this paper is too short to contain.)

Viewed as an N-lattice, the resulting structure can be described as a decoration[17] of the scaled standard lattice $2\mathbf{Z}_N$, with a basis consisting of the set of vectors given by all the integral linear combinations of the vector (7) and its 45 rotations through multiples of $2\pi/46$, with coefficients taken modulo 2. One can verify that modulo 2 there are just eleven such linearly independent vectors, and so the basis contains $2^{11} - 1 = 2047 = 89 \times 23$ nonzero vectors. We stress that this strange structure, like the decorations of the simple cubic lattice giving face-centered and body-centered cubic, yields a *lattice* —a set of points that looks the same regardless of which point it is viewed from—even though the size of the basis is rather larger than what one has come to expect from the crystallographic examples.

The other nonprincipal ideal of $\mathbf{Z}_{46}$ (there are two, since $h_{46} = 3$) is the direct sum of $2\mathbf{Z}_{46}$ and $\beta^* \mathbf{Z}_{46}$. Since complex conjugation is just a mirroring in the x axis, the two nonstandard lattices for $N = 46$ are, surprisingly, an enantiomorphic pair. (In the crystallographic case such pairs can be found among the three-dimensional *space groups*, but not even among the space groups in two dimensions.)

It is important for the development of a general quasicrystallographic classification scheme to realize that there are values of N (all but a finite number) for which there are nonstandard N-lattices that are *not* simply scaled and rotated versions of the obvious one, $\mathbf{Z}_N$. At the same time, it may some day prove useful to know those noncrystallographic values of N [Eq. (2)] other than 10 for which all lattices *are* equivalent to $\mathbf{Z}_N$.

It is splendid and remarkable that this enormous but (for physicists) arcane branch of number theory, developed in an effort to prove Fermat's last theorem, should contain precisely the structures needed to formulate and answer one of the most fundamental crystallographic questions raised by the discovery of quasicrystals.

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[1]D. S. Schechtman *et al.*, Phys. Rev. Lett. **53**, 1951 (1984).

[2]L. Bendersky, Phys. Rev. Lett. **55**, 1461 (1985).

[3]N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders College Publishing, Philadelphia, 1976), p. 70.

[4]This number, the *indexing dimension*, is given by the number of positive integers less than N (including 1) which are relatively prime to N.

[5]Daniel S. Rokhsar, N. David Mermin, and David C. Wright, Phys. Rev. B **35**, 5487 (1987).

[6]T. Ishimasa, H. U. Nissen, and Y. Fukano, Phys. Rev. Lett. **55**, 511 (1985).

[7]J. Myron Masley and Hugh L. Montgomery, J. Reine Angew. Math. **286**, 248 (1976).

[8]J. Myron Masley, Invent. Math. **28**, 243 (1975).

[9]J. M. Masley, in *Number Theory, Carbondale 1979,* edited by A. Dold and B. Eckmann (Springer-Verlag, New York, 1979).

[10]Lawrence Washington, *Introduction to Cyclotomic Fields* (Springer-Verlag, New York, 1982), Appendix 3.

[11]Ian Stewart and David Tall, *Algebraic Number Theory* (Chapman and Hall, London, 1979), Theorem 9.7, p. 165.

[12]See Harold M. Edwards, *Fermat's Last Theorem* (Springer-Verlag, New York, 1977), for a delightful historically oriented introduction to cyclotomic fields.

[13]We use $\mathbf{Q}_N$ and $\mathbf{Z}_N$ rather than the lengthier notation $\mathbf{Q}(\zeta_N)$ and $\mathbf{Z}(\zeta_N)$ prevalent in the mathematical literature. It is also the common practice of mathematicians to call ζ-integers simply "integers" in this context, using the term "rational integers" to refer to ordinary integers. Note, finally that when N is twice an odd number, the mathematicians always label things by $N/2$ rather than N.

[14]Ref. 11, p. 160.

[15]Ref. 10, p. 7.

[16]We are grateful to Keith Dennis for showing us how to do this.

[17]That any N-lattice can be viewed as such a decoration is the content of Theorem 5.14 of Stewart and Tall, Ref. 11, p. 126.