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LETTER TO THE EDITOR

Pseudo-crystal classes: counterexamples to Lomont's conjecture

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Abstract. It is shown that for spaces of dimensionality greater than three there exist pseudo-crystal classes of groups. Each element of such a group G appears in integral matrix form for some coordinate system but there exists no single coordinate system in which all elements of G appear simultaneously in integral form. These groups violate a long-standing conjecture of Lomont and bear a close affinity to the phenomenon of non-crystallographic long-range orientational order.

Perhaps the most elegant derivation of the 32 crystal classes in three dimensions (3D) is the group theoretical method of Frobenius (1911). Here the possible matrix operators are established by enumerating the possible irreducible factors of the characteristic polynomial. Each type of matrix operator is specified by its independent invariants, namely the trace or character $\chi(=\pm3, \pm2, \pm1, 0)$ and the determinant $d(=\pm1)$. The relations satisfied by group characters are then used to derive the possible orders for a crystallographic class. Finally using these same character relations and imposing the further restrictions that each class is a representation of type 1 (and, therefore, equivalent to a group of real matrices) the number $n(\chi, d)$ of group operators belonging to the symbol (χ, d) is obtained. The identification of each of the 32 crystal classes is then a simple matter.

Lomont (1959) discusses the 3D classes by a variant of Frobenius's method and, on the basis of these results and those in 2D and 1D spaces, makes the following general conjecture (Frobenius 1911, p 51).

Lomont's conjecture. A matrix group Γ is integral if Γ satisfies the three conditions:
(1) Γ is of the first kind,
(2) Γ has integral character,
(3) Γ is irreducible.

One attractive feature of Frobenius's method is that it appears, at first sight, to be applicable to spaces of any dimensionality. The sole complicating factor would seem to be the occurrence of additional invariants $\chi_2, \chi_3, \ldots, \chi_s$ in the characteristic equation of each matrix operator. Each of these higher invariants $\chi_2, \chi_3, \ldots, \chi_s$ is a generalised character χ of the crystal class (Murnaghan 1938) so that the standard character relations for a finite group may still be used to fix the possible orders of the classes and, for a given order, the distribution of the elements amongst the types $(\chi_1, \chi_2, \ldots, \chi_s)$ specified by the values of the s invariants.

Indeed the first part of the Frobenius program, the determination of all possible symmetry elements from the irreducible factors of the characteristic polynomial, goes through without difficulty for a space of any dimensionality and yields results in 4D in complete agreement with those obtained by other methods, each element being specified by three invariants (χ, σ, d) (Hurley 1950, Brown *et al* 1978).

However, when the second part of Frobenius's program was worked out in detail for the irreducible crystal classes in 4D, it proved impossible to reduce the number of solutions of the character relations below 70, even after the imposition of various *ad hoc* conditions from finite group theory, most of which were simple inferences from Sylow's theorems. Derivations by other methods (Hurley 1951, Brown *et al* 1978) show that there are, in fact, just 45 irreducible classes in 4D, leaving 25 solutions of the character relations unaccounted for. One might hope that a more thorough set of *ad hoc* conditions would eliminate these extraneous solutions and so restore the efficacity of Frobenius's method in 4D. However this too is impossible. As we show below, 3 of the 25 extraneous solutions correspond to finite groups of the first kind, which have integral values for all invariants (χ, σ, d), are irreducible, but are *not* integral groups (i.e. crystal classes). Clearly these groups are counterexamples to Lomont's conjecture. Furthermore, their existence precludes the possibility of a complete enumeration of the crystal classes in space of dimensionality greater than three by Frobenius's method, whatever *ad hoc* conditions from finite group theory are imposed.

The three counterexamples to Lomont's conjecture may be generated by 4D matrices a, b, c, d, f defined by the equations

$$a = \frac{1}{2}\begin{bmatrix} \sqrt{3} & -1 & 0 & 0 \\ 1 & \sqrt{3} & 0 & 0 \\ 0 & 0 & -\sqrt{3} & 1 \\ 0 & 0 & -1 & -\sqrt{3} \end{bmatrix} \qquad b = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

$$c = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} \qquad d = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \\ -1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \end{bmatrix}$$

$$f = \frac{1}{2}\begin{bmatrix} -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 \end{bmatrix}.$$

From these matrices we may construct two groups of order 48, G_{48} and G'_{48} and a group of order 144, G_{144}. Their generators, relations and elements are given by the following equations (with e the identity)

$$G_{48} = \langle a, b, c \rangle.$$

Relations $\quad a^{12} = e$

$$b^2 = e, \qquad ba = a^{11}b$$

$$c^2 = a^6, \qquad ca = a^7c, \qquad cb = bc.$$

Elements $\quad a^p b^q c^r \; (p = 0, 1, \ldots, 11;\; q, r = 0, 1)$

$G'_{48} = \langle a, b, d \rangle$

Relations $\quad a^{12} = e$

$b^2 = e, \qquad ba = a''b$

$d^2 = a^9, \qquad da = a^5 d, \qquad db = a^9 bd.$

Elements $\quad a^b b^q d^r \; (p = 0, 1, \ldots, 11;\; q, r = 0, 1)$

$G_{144} = \langle a, b, c, f \rangle.$

Relations $\quad a^{12} = e$

$b^2 = e, \qquad ba = a''b$

$c^2 = a^6, \qquad ca = a^7 c, \qquad cb = bc$

$f^3 = e, \qquad fa = a^4 cf, \qquad fb = a^3 bf, \qquad fc = a^3 cf.$

Elements $\quad a^p b^q c^r f^s \; (p = 0, 1, \ldots, 11;\; q, r = 0, 1;\; s = 0, 1, 2).$

It is straightforward to verify that the matrices a–f satisfy the above relations and that each of the groups G_{48}, G'_{48} and G_{144} satisfy all three conditions of Lomont's conjecture.

We now use *reductio ad absurdum* to show that none of the groups G_{48}, G'_{48}, G_{144} is integral.

If one of these groups is integral it must leave some 4D lattice L invariant.

Since L is 4D it must contain some vector

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \tag{1}$$

with $x_1 \neq 0$ and $x_3 \neq 0$.

Since b is an element of all three groups, the lattice L must contain the vector

$$y_1 = bx + x = \begin{bmatrix} 2x_1 \\ 0 \\ 2x_3 \\ 0 \end{bmatrix} = r \begin{bmatrix} \cos\theta \\ 0 \\ \sin\theta \\ 0 \end{bmatrix} \tag{2}$$

with

$$r \cos\theta \sin\theta \neq 0. \tag{3}$$

Since a is an element of all three groups, L must contain the vectors

$$y_2 = a y_1, \qquad y_3 = a^2 y_1, \qquad y_4 = a^3 y_1. \tag{4}$$

Direct evaluation gives

$$\det(y_1, y_2, y_3, y_4) = -3 r^4 \cos^2\theta \sin^2\theta, \tag{5}$$

so that, from (3), it follows that the vectors y_1, y_2, y_3, y_4 are linearly independent.

Using the matrix

$$S = (y_1, y_2, y_3, y_4) \tag{6}$$

to transform to a coordinate system with y_1, y_2, y_3, y_4 as basis vectors, we find that the transforms a', b', c', d', f' of the matrices a, b, c, d, f are given by the equations:

$$a' = S^{-1}aS = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \qquad b' = S^{-1}bS = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & -1 \end{bmatrix} \tag{7}$$

$$c' = S^{-1}cS = \tfrac{1}{2}(\tan\theta - \cot\theta)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

$$+\frac{1}{2\sqrt{3}}(\tan\theta + \cot\theta)\begin{bmatrix} 0 & -1 & 0 & 1 \\ 2 & 0 & 1 & 0 \\ 0 & -1 & 0 & -2 \\ -1 & 0 & 1 & 0 \end{bmatrix} \tag{8}$$

$$d' = S^{-1}dS = \frac{1}{2\sqrt{6}}(\tan\theta - \cot\theta)\begin{bmatrix} -1 & 2 & 1 & 1 \\ -2 & -1 & -1 & -2 \\ 2 & -1 & 1 & -2 \\ 1 & -1 & 2 & 1 \end{bmatrix}$$

$$+\frac{1}{2\sqrt{2}}(\tan\theta + \cot\theta)\begin{bmatrix} -1 & 0 & -1 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 \\ 1 & -1 & 0 & -1 \end{bmatrix} \tag{9}$$

$$f' = S^{-1}fS = \tfrac{1}{2}\begin{bmatrix} -1 & 1 & 0 & 1 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & -1 & 0 \\ -1 & 0 & -1 & -1 \end{bmatrix} + \tfrac{1}{4}(\tan\theta - \cot\theta)\begin{bmatrix} 1 & 1 & 0 & 1 \\ 0 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 1 & 0 & 1 & -1 \end{bmatrix}$$

$$+\frac{1}{4\sqrt{3}}(\tan\theta + \cot\theta)\begin{bmatrix} -1 & -1 & -2 & 1 \\ 2 & 1 & 1 & 2 \\ 2 & -1 & 1 & -2 \\ -1 & -2 & 1 & -1 \end{bmatrix}. \tag{10}$$

Since the basis vectors y_1, y_2, y_3, y_4 are lattice vectors, all elements of one of the matrix groups G_{48}, G'_{48}, G_{144} must appear in rational form for some choice of θ satisfying (3). For the groups $G_{48} = \langle a', b', c'\rangle$ and $G_{144} = \langle a', b', c', f'\rangle$ this implies, from equations (8) and (10), that $(\tan\theta - \cot\theta)$ and $(1/\sqrt{3})(\tan\theta + \cot\theta)$ are both rational for some value of θ, whilst for $G'_{48} = \langle a, b, d\rangle$ this implies, from equation (9), that $(1/\sqrt{6})\times(\tan\theta - \cot\theta)$ and $(1/\sqrt{2})(\tan\theta + \cot\theta)$ are both rational for some value of θ. These conditions reduce to the Diophantine equations

$$x^2 + y^2 = 3t^2 \tag{11}$$

and

$$2x^2 + 3y^2 = t^2 \tag{12}$$

respectively, for integers x, y and t.

However, a simple parity argument (Hardy and Wright 1954) shows that equations (11) and (12) have no integer solutions. We therefore have a contradiction and our original assumption of the existence of the lattice L is disproved; none of the groups G_{48}, G'_{48} and G_{144} is integral.

It is of some interest that, if complex values are admitted for the coordinates, equations (11) and (12) have obvious solutions in terms of Gaussian integers of the form $p+iq$ with p and q natural integers. These in turn allow us to express all generators of each of the groups G_{48}, G'_{48} and G_{144} as Gaussian rationals. Indeed, for each group, the matrices of all elements appear in terms of Gaussian rationals, which can easily be transformed into Gaussian integers if need be. For example if, in equations (8) and (10), we choose $\tan\theta-\cot\theta=\mathrm{i}$, $\tan\theta+\cot\theta=\sqrt{3}$, which is consistent with $\tan\theta\cot\theta=1$, we obtain

$$c'=\frac{1}{2}\begin{bmatrix} \mathrm{i} & -1 & 0 & 0 \\ 2 & -\mathrm{i} & 1 & 0 \\ 0 & -1 & \mathrm{i} & -2 \\ -1 & 0 & 1 & -\mathrm{i} \end{bmatrix} \qquad f'=\frac{1}{4}\begin{bmatrix} -3+\mathrm{i} & 1+\mathrm{i} & -2 & 3+\mathrm{i} \\ 2 & -1-\mathrm{i} & 3-\mathrm{i} & 2 \\ 2 & -3-\mathrm{i} & -1+\mathrm{i} & -2 \\ -3+\mathrm{i} & -2 & -1+\mathrm{i} & -3-\mathrm{i} \end{bmatrix} \tag{13}$$

so that all elements of $G_{48}=\langle a', b', c'\rangle$ and $G_{144}=\langle a', b', c', f'\rangle$ appear in terms of Gaussian rationals. Of course, the invariants (χ, σ, d) remain unchanged as natural integers.

Similarly, if we choose $(1/2\sqrt{6})(\tan\theta-\cot\theta)=\frac{1}{2}\mathrm{i}$ and $(1/2\sqrt{2})(\tan\theta+\cot\theta)=\frac{1}{2}\mathrm{i}$ in equation (9), all elements of G'_{48} appear as Gaussian rationals, and may easily be transformed to Gaussian integral form.

Since G_{48}, G'_{48} and G_{144} are the only 4D matrix groups which violate Lomont's conjecture (Hurley 1951) we see that, at least for dimensionalities less than 5, the truth of the conjecture may be reinstated by allowing Gaussian integers as well as natural integers in the integral matrix group. The number of complex, geometric crystal classes then becomes 230, the same as the number of real space groups in 3D. A curious coincidence?

In spaces of dimensionality greater than 4 it seems likely that Gaussian integers may not suffice. Instead we advance the

Revised Lomont conjecture. If a matrix group Γ is of the first kind, has integral character and is irreducible, then, in a suitable coordinate system, all matrix elements of all operators in Γ appear as algebraic integers.

We note that, for a matrix *group*, integral characters guarantee integral values for all invariants. This is because the higher invariants are integral functions of the traces of the powers of the matrix (Murnaghan 1938).

The physical significance of these exceptional groups is not at present clear, although they show some striking affinities to the quasi-crystalline translations and rotations involved in non-crystallographic long-range orientational order. There too one encounters operators (translational), each of which appears integral in some coordinate system, but there is no single coordinate system in which all operators are integral simultaneously, as is the case for a space group (Levine and Steinhardt 1984, Schechtman *et al* 1984).

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