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Sublattice enumeration. IV. Equivalence classes of plane sublattices by parent Patterson symmetry and colour lattice group type

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The Dirichlet generating functions for the number of sublattices fixed under each symmetry operation of the parent Patterson group may be combined to count the number of crystallographically nonequivalent sublattices, in total, by sublattice point group and by colour lattice group type. The combinatorial formulae used imply the existence of various congruences among the corresponding arithmetic functions.

1. Introduction

The original article in this series[1] (Rutherford, 1992) dealt with the enumeration, using number theoretical methods, of the sublattices of a parent lattice that are consistent with the parent structure and a derived structure belonging to the same crystal class. Since the intention was to make the work relevant to crystal structures rather than the abstract mathematical lattice, only those sublattices that maintained the relevant symmetry operations of the parent lattice were considered. For example, a sublattice was considered cubic only if it maintained the orientation of the axes present in the parent cubic lattice, and 'inclined cubic' lattices (Frei, 1990) were not included.

Currently there is renewed interest in counting the number of derivative structures (or commensurate superlattices in the terms favoured by physicists) that may arise from some aristotype. For example, Hart & Forcade (2008) have developed an improved algorithm to identify such structures. The present article is intended to support these endeavours in providing a closed-form enumeration of these structures in the two-dimensional case, and indicating how the same might be done in three dimensions.

There are two major aspects to this work, the first being the study of symmetry. The subgroups of the crystallographic plane groups were discussed in detail by Senechal (1979), and the invariant subgroups in particular completely classified in a subsequent article (Senechal, 1985). In particular, in the latter Senechal tabulated the various types of such subgroups $\mathcal{H}$ of finite index in the plane group $\mathcal{G}$, which are the cases of interest to us, in terms which included the form of their translational subgroups $\mathcal{T}_{\mathcal{H}}$ as a 2×2 matrix defining the basis vectors, and $\mathcal{T}_{\mathcal{G}}/\mathcal{T}_{\mathcal{H}}$, the translational factor group, essentially equivalent to the colour lattice group described below.

This work in turn led to a unified description of derivative structures – crystal structures based on a sublattice **S**, where individual unit cells of an underlying lattice $\boldsymbol{\Lambda}$ vary in a regular manner in composition, atomic positions or spin – developed by Kucab (1981) and Rolley-Le Coz *et al.* (1983), who based their descriptions on the colour lattice, in which the lattice points of $\boldsymbol{\Lambda}$ are assigned colours to represent the property in question. Both these articles recognize that the key to such a description lies in the structure of the finite Abelian group $\mathcal{A}$ associated with this colour lattice, described by Harker (1978) as consisting of a direct product of cyclic groups

$$\mathcal{A} \cong \times_{i=1}^{j} \mathcal{C}_{n_i} \quad 1 \le j \le D; \quad n_{i+1} | n_i,$$

where D is the dimension of the lattice.

$\mathcal{A}$ has variously been called the *colour translation group* or the *colour lattice group*, according to Lifshitz (1997), who idiosyncratically names it the *lattice colour group*. Since the term colour translation group in D dimensions would more naturally refer to $\mathcal{A} \times \mathcal{T}_D$, by analogy with the use of colour space group and colour point group, we shall continue the practice of Rutherford (1993), which dealt with the distribution of sublattices among the isomorphism classes, in calling them colour lattice groups.

De Las Peñas & Felix (2007) continued this line of investigation with specific regard to the colouring of sublattices, analysing the sublattices of the square and hexagonal plane lattices in terms of the combination of point group and colour lattice group that characterizes each sublattice.

The other major aspect that concerns us is the enumeration of crystallographic objects using Dirichlet generating functions. Rutherford (1992) applied such functions to enumerate sublattices that maintained the symmetry of the parent lattice. This was then followed by enumeration by colour lattice group for a general lattice (Rutherford, 1993).

[1] The series title has now been changed from that used in previous articles, namely *The enumeration and symmetry-significant properties of derivative lattices*, to reflect the relevance to sublattices, since the previous articles were largely overlooked by subsequent authors. See, for example, Gruber (1997).

More recently du Sautoy *et al.* (1999) examined the distribution by index of the subgroups of the crystallographic plane groups, the so-called subgroup growth problem, and derived the group zeta-functions, *i.e.* the Dirichlet generating functions for these numbers. However, their generating functions present a problem when applied in a typical crystallographic context, since they combine together subgroups of a given index indiscriminately. In contrast, we choose to maintain the usual distinction of classifying minimal crystallographic group–subgroup relations – the individual steps in descent in symmetry from an aristotype through a Bärnighausen (1980) tree – as being either of the translation-equivalent or the class-equivalent type. In this way we may temporarily set aside the translation-equivalent steps in such a tree and enumerate only the nonequivalent sublattices, and assign to each such sublattice a point symmetry which is maximal for any structure that adopts that sublattice. The true index of such a structure in the aristotype will be the product of the index of its lattice in the parent lattice times the index of the point group of its structure in the point group of the parent structure.

This enumeration is based on the concept of the parent lattice being associated with a specific Patterson symmetry. The Patterson symmetry of a crystal structure, that is, the symmetry of its self-convolution function, is that of the centrosymmetric and symmorphic space group which otherwise corresponds to the actual space group of the structure (Hahn & Looijenga-Vos, 2002). Since the underlying lattice is also centrosymmetric and symmorphic, it has this same symmetry group. Hence we classify the sublattices of given index n into equivalence classes under the point operations of this parent symmetry, as shown in Fig. 1.

In the case of the plane groups, this reduces the number of cases from 17 to 7; for example, the primitive rectangular plane groups *pm*, *pg*, *p*2*mm*, *p*2*mg* and *p*2*gg* all correspond to Patterson symmetry *p*2*mm*.

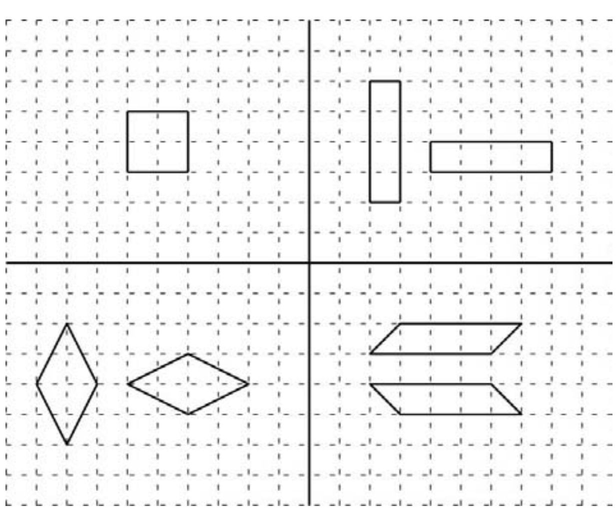

Figure 1
The unit cells of the seven index-4 sublattices of the square lattice, partitioned into the four equivalence classes under parent *p*4*mm*.

We shall also have cause to refer to some integer sequences relevant to our problem which have been published in Sloane (2008).

2. Effect of parent symmetry

The full group of any plane lattice will include the two-dimensional translation group $\mathcal{T}_2$ as a subgroup. Hence we can classify the full group Γ of any plane lattice as a semidirect product

$$\Gamma = \mathcal{P} \rtimes \mathcal{T}_2$$

where $\mathcal{P}$ is a finite point group which may include the symmetry-operator types 1, 2, 3, 4 and m.

We then apply a standard approach from combinatorics, the orbit-counting theorem, also called Burnside's lemma (Burnside, 1897), where we enumerate the objects (here sublattices) that are fixed by each operation of the group (*i.e.* $\mathcal{P}$) and average them. This yields

$$F_{\mathcal{P}}(s) = (1/|\mathcal{P}|) \sum_{g \in \mathcal{P}} F_g(s), \qquad (1)$$

where $F_{\mathcal{P}}(s)$ is the total generating function for distinct sublattices of norm n and $F_g(s)$ is the function counting sublattices fixed under the class of operation $g \in \mathcal{P}$. The $F_g(s)$ are Dirichlet generating functions, that is they are formal series of the type

$$F_g(s) = \sum_{n=1}^{\infty} f_g(n) n^{-s}, \qquad (2)$$

where $f_g(n)$ is an arithmetic function multiplicative in the primes, *i.e.*

$$f_g(mn) = f_g(m) f_g(n),$$

provided (m, n) are mutually prime.

We next note that the minimum symmetry of a plane lattice is actually *p*2, and that the symmetry elements of each group $\mathcal{P}$ can be broken down into coset pairs

$$g_i = 2 \cdot g_j$$

which have the same effect on the lattice. In particular, the twofold rotation is equivalent to the identity operation. Thus we may reduce the number of terms in equation (1) by half, and write

$$F_{\mathcal{P}}(s) = (2/|\mathcal{P}|) \sum_{i=1}^{|\mathcal{P}|/2} F_i(s), \qquad (3)$$

where the sum is now over only those symmetry elements which differ in effect.

The generating functions for sublattices fixed by the possible symmetry elements are collected as entries (*a*) to (*e*) in Table 1; as these each correspond to a set of sublattices of fixed symmetry, they have been taken directly from Rutherford (1992), but with m_c and some nomenclature corrected. Here the label m_p represents a mirror plane fixing a primitive rectangular lattice and m_c a centred one.

Table 1
Generating functions for the number of sublattices fixed by the various types of point operations acting on the plane, with the coefficients of the first 30 terms.

		n									
		1	2	3	4	5	6	7	8	9	10
		11	12	13	14	15	16	17	18	19	20
Label and operator	Generating function	21	22	23	24	25	26	27	28	29	30
(*a*)	$\zeta(s)\zeta(s-1)$	1	3	4	7	6	12	8	15	13	18
1 or 2		12	28	14	24	24	31	18	39	20	42
		32	36	24	60	31	42	40	56	30	72
(*b*)	$\zeta(s)L(s, \chi_3)$	1	0	1	1	0	0	2	0	1	0
3		0	1	2	0	0	1	0	0	2	0
		2	0	0	0	1	0	1	2	0	0
(*c*)	$\zeta(s)L(s, \chi_4)$	1	1	0	1	2	0	0	1	1	2
4		0	0	2	0	0	1	2	1	0	2
		0	0	0	0	3	2	0	0	2	0
(*d*)	$(1+2^{-s})\zeta^2(s)$	1	3	2	5	2	6	2	7	3	6
$m_{\rm p}$		2	10	2	6	4	9	2	9	2	10
		4	6	2	14	3	6	4	10	2	12
(*e*)	$(1-2^{-s}+2.4^{-s})\zeta^2(s)$	1	1	2	3	2	2	2	5	3	2
$m_{\rm c}$		2	6	2	2	4	7	2	3	2	6
		4	2	2	10	3	2	4	6	2	4

The actual calculations are more simply based on the corresponding arithmetic functions, which are as follows:

$$
\begin{array}{lll}
(a) & \sigma_1(n) & \\
(b) & r_H(n)/6 & \\
(c) & r(n)/4 & \\
(d) & \sigma_0(n) & 2\not|\, n \\
 & \sigma_0(n)+\sigma_0(n/2) & 2|n \\
(e) & \sigma_0(n) & 2\not|\, n \\
 & \sigma_0(n)-\sigma_0(n/2) & 2|n, 4\not|\, n \\
 & \sigma_0(n)-\sigma_0(n/2)+2\sigma_0(n/4) & 4|n,
\end{array}
$$

where $\sigma_0(n)$ is the number of divisors function, $\sigma_1(n)$ is the sum of divisors function, r is the number of representations of n as the sum of two squares and r_H is the number of representations of n of the form h^2+hk+k^2. The results of applying equation (1) for the various plane Patterson symmetries are given in Table 2.

3. Sublattice point symmetry

We now consider the distribution of these nonequivalent sublattices by point symmetry. The key here is that the orbit-counting theorem may be considered to be based on the reducible representation of the set $\mathcal{S}$, here the set of sublattices $\mathcal{S}$ of index n, under the action of the group $\mathcal{P}$. In this interpretation the Burnside formula simply counts the number of occurrences of Γ_1, the totally symmetric representation, in the representation of $\mathcal{S}$, and, since Γ_1 occurs once in the representation of each orbit, it thereby counts the orbits.

Since we require the sublattices to be invariant to a twofold rotation in the plane, those irreducible representations Γ_i, $i = 1, \ldots s$, that are symmetric with respect to this operation are sufficient to form an orthogonal basis for the representation $\Gamma_{\mathcal{S}}$ of the set of sublattices $\mathcal{S}$ under the action of the group $\mathcal{P}$.

In turn each relevant orbit class O_j, where $j = 1, \ldots t$ and t is the number of orbit classes of $\mathcal{P}$, has a (generally reducible) representation given by

$$\Gamma(O_j) = \Gamma_1 + \sum_{k=2}^{r} M_{jk}\Gamma_k,$$

where we have included the fact that the totally symmetric representation appears once in the representation of each orbit class.

Now, since the orbits partition $\mathcal{S}$ uniquely, provided $s = t$ we can determine a square matrix $\mathbf{N}$ such that

$$\mathbf{n}_o = \mathbf{N}\mathbf{n}_{\mathcal{S}}, \qquad (4)$$

where $n_o(i)$ is the number of orbits of class i and $n_{\mathcal{S}}(k)$ is the number of sublattices fixed by symmetry operation k. This holds true for $p2$ (trivial, as $s = t = 1$), and for $p2mm$,[2] $c2mm$, $p4$ and $p6$, for which $s = t = 2$.

In the $s = 2$ cases, there can be no ambiguity in labelling the irreducible representations, and the results follow immediately. For plane groups $\mathcal{G} \cong p2mm$, $c2mm$ or $p4$ we have

$$\begin{pmatrix} n_O(\mathcal{G}) \\ n_O(p2) \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & 2 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} f_E \\ f_g \end{pmatrix},$$

[2] A sublattice of parent *p2mm* may be *p2mm* or *c2mm*, as also can a sublattice of parent *c2mm*, depending on its index and colour lattice group.

Table 2
Generating functions for the number of nonequivalent sublattices for the plane Patterson symmetries, with the coefficients for the first 30 terms.

		n									
		1	2	3	4	5	6	7	8	9	10
		11	12	13	14	15	16	17	18	19	20
Symmetry	Generating function	21	22	23	24	25	26	27	28	29	30
*p*2	(a)	1	3	4	7	6	12	8	15	13	18
		12	28	14	24	24	31	18	39	20	42
		32	36	24	60	31	42	40	56	30	72
*p*2*mm*	$\frac{1}{2}(a+d)$	1	3	3	6	4	9	5	11	8	12
		7	19	8	15	14	20	10	24	11	26
		18	21	13	37	17	24	22	33	16	42
*c*2*mm*	$\frac{1}{2}(a+e)$	1	2	3	5	4	7	5	10	8	10
		7	17	8	13	14	19	10	21	11	24
		18	19	13	35	17	22	22	31	16	38
*p*4	$\frac{1}{2}(a+c)$	1	2	2	4	4	6	4	8	7	10
		6	14	7	12	12	16	10	20	10	22
		16	18	12	30	17	22	20	28	16	36
*p*4*mm*	$\frac{1}{4}(a+c+d+e)$	1	2	2	4	4	5	3	7	5	7
		4	11	5	8	8	12	6	13	6	15
		10	11	7	21	10	13	12	18	9	22
*p*6	$\frac{1}{3}(a+2b)$	1	1	2	3	2	4	4	5	5	6
		4	10	6	8	8	11	6	13	8	14
		12	12	8	20	11	14	14	20	10	24
*p*6*mm*	$\frac{1}{6}(a+2b+3e)$	1	1	2	3	2	3	3	5	4	4
		3	8	4	5	6	9	4	8	5	10
		8	7	5	15	7	8	9	13	6	14

where the subscript g denotes the relevant operation (m or 4) of $\mathcal{P}$, and for *p*6

$$\begin{pmatrix} n_O(p6) \\ n_O(p2) \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 0 & 3 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} f_E \\ f_3 \end{pmatrix}.$$

However, *p*4*mm* and *p*6*mm* have more orbit classes than irreducible representations; this is resolved for *p*4*mm*, where the point-group operations are E, 4, m_1 and m_2, and the orbit classes are *p*4*mm*, *p*4, $*2mm_1$ (the asterisk is used here because the orbit class contains sublattices of both types *p*2*mm* and *c*2*mm*), $*2mm_2$ and *p*2, as follows. Equation (1) has here the explicit form

$$F_{p4mm} = (1/4)(F_E + F_4 + F_{m_1} + F_{m_2}). \qquad (5)$$

We first note that additional information is available, in that we may also write a generating function for the number of sublattices fixed by all the operations of the point group 4*mm*,

$$F_{4mm} = (1 + 2^{-s})\zeta(2s) = 1 + 2^{-s} + 4^{-s} + 8^{-s} + 9^{-s} + \ldots, \qquad (6)$$

and that this number can only be 0 or 1. As a result, there can only be one valid solution in terms of all n_j being non-negative integers, as the following illustrates.

Table 3 provides an extract from the character table of point group 4*mm* (C_{4v}) taken from Kettle (1995). As discussed above, we only need to consider those representations that are symmetric under C_2, hence a fifth irreducible representation, E, has been omitted as irrelevant to our calculations. Now, making an arbitrary choice between the mirror operations σ and σ', the representations of the orbit classes are as follows:

$$\begin{aligned} \Gamma(p4mm) &= A_1 \\ \Gamma(p4) &= A_1 + A_2 \\ \Gamma(*mm_1) &= A_1 + B_2 \\ \Gamma(*mm_2) &= A_1 + B_1 \\ \Gamma(p2) &= A_1 + A_2 + B_1 + B_2. \end{aligned}$$

Now all the representations of any orbit class other than *p*4*mm* contain an even number of irreducible representations each of order 1, for which each character $\chi_g = \pm 1$. It follows that each character in the representation of that class is an even integer, and that each character in the total set of sublattices of index n is even, save for any contribution from an orbit of class *p*4*mm*. Since, in turn, there can be at most one sublattice of index n fixed by all the operations of point group 4*mm*, the individual terms in equation (5) must either be all odd or all even, and have the parity of the corresponding term, one or zero, in the series of equation (6).

Thus we may subtract the term in equation (6) from each of the terms in equation (5) to give resulting terms that are always even, and use that result to count the other four possible orbit classes.

In these cases (*p*4*mm* and *p*6*mm*) the square matrix that takes the role of **N** has the form

Table 3
An extract from the character table of point group $4mm$.

	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma'_v$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	−1	1	1	−1
B_2	1	−1	1	−1	1

$$\left(\begin{array}{c|ccc} 1 & 0 & 0 & \dots \\ \hline -1 & & & \\ -1 & & \mathbf{Q} & \\ \vdots & & & \end{array}\right).$$

Writing only **Q**, which derives from the irreducible representations, explicitly, we have for $p4mm$

$$\begin{pmatrix} n_O(p4) \\ n_O(*2mm_1) \\ n_O(*2mm_2) \\ n_O(p2) \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \\ 1 & -1 & -1 & -1 \end{pmatrix}\begin{pmatrix} f_E - f_{4mm} \\ f_4 - f_{4mm} \\ f_{m_1} - f_{4mm} \\ f_{m_2} - f_{4mm} \end{pmatrix}.$$

The parent point group $p6mm$ may be treated in a similar fashion, with

$$F_{6mm} = (1 + 3^{-s})\zeta(2s) = 1 + 3^{-s} + 4^{-s} + 9^{-s} + 12^{-s} + \dots \quad (7)$$

and $f_E(n)$ being congruent modulo 2 with f_m and modulo 3 with f_6. The process already outlined for $p4mm$ yields

$$\begin{pmatrix} n_O(p6) \\ n_O(*2mm) \\ n_O(p2) \end{pmatrix} = \frac{1}{6}\begin{pmatrix} 0 & 3 & 0 \\ 0 & 0 & 6 \\ 1 & -1 & -3 \end{pmatrix}\begin{pmatrix} f_E - f_{6mm} \\ f_6 - f_{6mm} \\ f_m - f_{6mm} \end{pmatrix}.$$

4. Colour lattice group

The other aspect of the symmetry of the sublattice we need to identify is its colour lattice group. Only one colour lattice group, namely the cyclic group C_n, occurs if the index n is square-free, *i.e.* has no repeated prime factors, but if it is not square-free, more than one colour lattice group will occur for that n. The number of sublattices belonging to each colour lattice group for given n was derived in Rutherford (1993) by Möbius inversion, a technique which also may be applied here.

We take a generating function, $F_{\mathcal{P}}(s)$, a linear combination of multiplicative functions, which counts all relevant sublattices irrespective of their colour lattice group. We then define $F'_{\mathcal{P}}(s)$ as the corresponding generating function for sublattices with colour lattice group C_n. For each such sublattice there is another with index nm^2 and colour lattice group $C_{mn} \times C_m$ for any m, and so the coefficients $f_{\mathcal{P}}(n)$ and $f'_{\mathcal{P}}(n)$ of these two series are related by

$$f_{\mathcal{P}}(n) = \sum_{m^2|n} f'_{\mathcal{P}}(n/m^2). \quad (8)$$

Hence

$$F_{\mathcal{P}}(s) = \zeta(2s)F'_{\mathcal{P}}(s),$$

which implies

$$F'_{\mathcal{P}}(s) = \zeta^{-1}(2s)F_{\mathcal{P}}(s),$$

where

$$\zeta^{-1}(2s) = \sum_{n=1}^{\infty} \mu(n)n^{-2s} = 1 - 4^{-s} - 9^{-s} - 25^{-s} + 36^{-s} \dots.$$

$\mu(n)$ is the Möbius function, for which $\mu(a) = 1$ if $a = 1$, $\mu(a) = (-1)^r$ if a is the product of r distinct prime factors, *i.e.* if a is square-free, and $\mu(a) = 0$ otherwise, *i.e.* if a is divisible by the square of a prime.

It is by this means that one may isolate the individual terms in equation (8). This in turn allows a complete breakdown of the equivalence classes of sublattices by symmetry (Tables 4 and 5).

5. Discussion

5.1. Interpreting the tables

Let us consider the index 28 sublattices of a parent structure in $p4mm$. From Table 1 we may determine the relevant Dirichlet generating functions for the point operations of $4mm$, while from Table 2 we find that the total number of sublattices of index 28, $\sigma_1(28) = 56$, break down into 18 equivalence classes. Table 5 tells us that these 18 classes comprise, for colour lattice group C_{28}, four classes of rectangular sublattices with mirror planes parallel to the axes of the parent, two classes of rectangular lattices with the diagonal orientation, and nine classes of oblique sublattices, while for group $C_{14} \times C_2$ we have one class in each of these three categories.

A crystal structure whose lattice belongs to any of the eight rectangular classes will have minimum overall index 56 relative to the parent, and, if it belongs to any of the ten oblique classes, 112.

Rutherford (1995) provides a method to count the number of possible structures, treated as colourings of the lattice, based on index and colour lattice group.

5.2. Integer sequences

$\sigma_1(n)$ appears as Sloane (2008) sequence A000203, and the sequence of equation (6) as both the Dirichlet generating function (A093709) and as A028982 in the form

$$1, 2, 4, 8, 9, 16, \dots.$$

However, in addition, the sequences formed from the coefficients for $p4$, $p4mm$, $p6$ and $p6mm$ differ, although only in detail, from similar sequences also listed by Sloane. The differences arise because Sloane only considers the metrics in comparing sublattices, and not their precise equivalence in terms of the arrangement of the interior points of their cosets, and so treats rotations of other than the crystallographic $(2\pi/n)$ types to be valid equivalences. The three sublattices in Fig. 2, where

Table 4
Numbers of equivalence classes of sublattices for parents $p2$, $p2mm$, $c2mm$, $p4$ and $p6$.

For columns 3 to 11, the first row of the column heading shows the parent symmetry and the second row shows the sublattice symmetry.

		$p2$	$p2mm$		$c2mm$		$p4$		$p6$	
n	Colour lattice group type	$p2$	$*mm$	$p2$	$*mm$	$p2$	$p4$	$p2$	$p6$	$p2$
2	C_2	3	3	0	1	1	1	1	0	1
3	C_3	4	2	1	2	1	0	2	1	1
4	C_4	6	4	1	2	2	0	3	0	2
	$C_2 \times C_2$	1	1	0	1	0	1	0	1	0
5	C_5	6	2	2	2	2	2	2	0	2
6	C_6	12	6	3	2	5	0	6	0	4
7	C_7	8	2	3	2	3	0	4	2	2
8	C_8	12	4	4	4	4	0	6	0	4
	$C_4 \times C_2$	3	3	0	1	1	1	1	0	1
9	C_9	12	2	5	2	5	0	6	0	4
	$C_3 \times C_3$	1	1	0	1	0	1	0	1	0
10	C_{10}	18	6	6	2	8	2	8	0	6
11	C_{11}	12	2	5	2	5	0	6	0	4
12	C_{12}	24	8	8	4	10	0	12	0	8
	$C_6 \times C_2$	4	2	1	2	1	0	2	1	1
13	C_{13}	14	2	6	2	6	2	6	2	4
14	C_{14}	24	6	9	2	11	0	12	0	8
15	C_{15}	24	4	10	4	10	0	12	0	8
16	C_{16}	24	4	10	4	10	0	12	0	8
	$C_8 \times C_2$	6	4	1	2	2	0	3	0	2
	$C_4 \times C_4$	1	1	0	1	0	1	0	1	0
17	C_{17}	18	2	8	2	8	2	8	0	6
18	C_{18}	36	6	15	2	17	0	18	0	12
	$C_6 \times C_3$	3	3	0	1	1	1	1	0	1
19	C_{19}	20	2	9	2	9	0	10	2	6
20	C_{20}	36	8	14	4	16	0	18	0	12
	$C_{10} \times C_2$	6	2	2	2	2	2	2	0	2
21	C_{21}	32	4	14	4	14	0	16	2	10
22	C_{22}	36	6	15	2	17	0	18	0	12
23	C_{23}	24	2	11	2	11	0	12	0	8
24	C_{24}	48	6	21	8	20	0	24	0	16
	$C_{12} \times C_2$	12	8	2	2	5	0	6	0	4
25	C_{25}	30	2	14	2	14	2	14	0	10
	$C_5 \times C_5$	1	1	0	1	0	1	0	1	0
26	C_{26}	42	6	18	2	20	2	20	0	14
27	C_{27}	36	2	17	2	17	0	18	0	12
	$C_9 \times C_3$	4	2	1	2	1	0	2	1	1
28	C_{28}	48	4	22	4	22	0	24	0	16
	$C_{14} \times C_2$	8	6	1	2	3	0	4	2	2
29	C_{29}	30	2	14	2	14	2	14	0	10
30	C_{30}	72	12	30	4	34	0	36	0	24

$$(a) = \begin{bmatrix} 5 & 0 \\ 0 & 5 \end{bmatrix},\ (b) = \begin{bmatrix} 25 & 0 \\ -7 & 1 \end{bmatrix} \text{ and } (c) = \begin{bmatrix} 25 & 0 \\ 7 & 1 \end{bmatrix},$$

are thus considered equivalent, although they clearly differ in the arrangement of the interior points (the open circles). Sublattices (*b*) and (*c*) – which would be 'inclined square' sublattices in the terminology of Frei (1990) – are only equivalent to each other as sublattices of a $p4mm$ parent, and not of a $p4$ parent, while sublattice (*a*) is unique in both cases. In general the points of difference may be identified using sequences (*b*) and (*c*) of Table 1, as detailed below.

(1) A054345. Number of inequivalent sublattices of index n in a square lattice, where two lattices are considered equivalent if one can be rotated to give the other. Identical to $p4$ except when $(c) > 1$.

(2) A054346. Number of inequivalent sublattices of index n in a square lattice, where two lattices are considered equivalent if one can be rotated and/or reflected to give the other. Identical to $p4mm$ except when $(c) > 2$.

(3) A054384. Number of inequivalent sublattices of index n in a hexagonal lattice, where two lattices are considered equivalent if one can be rotated to give the other. Identical to $p6$ except when $(b) > 1$.

(4) A003051. Number of inequivalent sublattices of index n in a hexagonal lattice, where two lattices are considered equivalent if one can be rotated and/or reflected to give the other. Identical to $p6mm$ except when $(b) > 2$, which first occurs for $n = 49$.

5.3. Asymptotic estimation

Hart & Forcade (2008) note that the number of equivalence classes of sublattices, as a fraction of the total number of sublattices, tends to $2/|\mathcal{P}|$ from above with increasing n.

Table 5
Numbers of equivalence classes of sublattices for parents $p4mm$ and $p6mm$.

For columns 3 to 11, the first row of the column heading shows the parent symmetry and the second row shows the sublattice symmetry.

		$p4mm$					$p6mm$			
n	Colour lattice group type	$p4mm$	$p4$	$*mm_1$	$*mm_2$	$p2$	$p6mm$	$p6$	$*mm$	$p2$
2	C_2	1	0	1	0	0	0	0	1	0
3	C_3	0	0	1	1	0	1	0	1	0
4	C_4	0	0	2	1	0	0	0	2	0
	$C_2 \times C_2$	1	0	0	0	0	1	0	0	0
5	C_5	0	1	1	1	0	0	0	2	0
6	C_6	0	0	3	1	1	0	0	2	1
7	C_7	0	0	1	1	1	0	1	2	0
8	C_8	0	0	2	2	1	0	0	4	0
	$C_4 \times C_2$	1	0	1	0	0	0	0	1	0
9	C_9	0	0	1	1	2	0	0	2	1
	$C_3 \times C_3$	1	0	0	0	0	1	0	0	0
10	C_{10}	0	1	3	1	2	0	0	2	2
11	C_{11}	0	0	1	1	2	0	0	2	1
12	C_{12}	0	0	4	2	3	0	0	4	2
	$C_6 \times C_2$	0	0	1	1	0	1	0	1	0
13	C_{13}	0	1	1	1	2	0	1	2	1
14	C_{14}	0	0	3	1	4	0	0	2	3
15	C_{15}	0	0	2	2	4	0	0	4	2
16	C_{16}	0	0	2	2	4	0	0	4	2
	$C_8 \times C_2$	0	0	2	1	0	0	0	2	0
	$C_4 \times C_4$	1	0	0	0	0	1	0	0	0
17	C_{17}	0	1	1	1	3	0	0	2	2
18	C_{18}	0	0	3	1	7	0	0	2	5
	$C_6 \times C_3$	1	0	1	0	0	0	0	1	0
19	C_{19}	0	0	1	1	4	0	1	2	2
20	C_{20}	0	0	4	2	6	0	0	4	4
	$C_{10} \times C_2$	0	1	1	1	0	0	0	2	0
21	C_{21}	0	0	2	2	6	0	1	4	3
22	C_{22}	0	0	3	1	7	0	0	2	5
23	C_{23}	0	0	1	1	5	0	0	2	3
24	C_{24}	0	0	4	4	8	0	0	8	4
	$C_{12} \times C_2$	0	0	3	1	1	0	0	2	1
25	C_{25}	0	1	1	1	6	0	0	2	4
	$C_5 \times C_5$	1	0	0	0	0	1	0	0	0
26	C_{26}	0	1	3	1	8	0	0	2	6
27	C_{27}	0	0	1	1	8	0	0	2	5
	$C_9 \times C_3$	0	0	1	1	0	1	0	1	0
28	C_{28}	0	0	4	2	9	0	0	4	6
	$C_{14} \times C_2$	0	0	1	1	1	0	1	2	0
29	C_{29}	0	1	1	1	6	0	0	2	4
30	C_{30}	0	0	6	2	14	0	0	4	10

If we call the average value of this fraction R, it is given by

$$R = \lim_{n\to\infty} \overline{\left\{\left[(2/|\mathcal{P}|)\sum_{i=1}^{|\mathcal{P}|/2} f_i\right] \Big/ f_E(D)\right\}},$$

where $f_E(D)$ is the total number of sublattices in D dimensions given by the expansion of $\prod_{i=1}^{D} \zeta(s-D+1)$ (Rutherford, 1992).

We next split off the term corresponding to identity operation E from the others in the numerator:

$$R = (2/|\mathcal{P}|)\left[1 + \lim_{n\to\infty} \overline{\left\{\left(\sum_{i=2}^{|\mathcal{P}|/2} f_i\right) \Big/ f_E(D)\right\}}\right].$$

Since its denominator has asymptotic density proportional to n^{D-1}, the second term within the square brackets will be asymptotically zero unless at least one of the terms in the numerator is also proportional to *exactly* n^{D-1}. (Any exponent greater than this leads to $R > 1$, a contradiction.) Such a term in turn would have $\zeta(s-D+1)$ as a factor in its generating function (Knopfmacher, 1990). It may be shown exhaustively that no symmetry operation in two or three dimensions, other than the identity operation, has the required properties, and hence

$$R = 2/|\mathcal{P}|.$$

5.4. Congruences

Since the various formulae above involve a division by the group order, the corresponding arithmetic functions must sum to 0 modulo ($|\mathcal{P}|/2$). This in turn results in the following congruences:

(1)

$$f_E(n) \equiv f_4(n) \equiv f_{m_p}(n) \equiv f_{m_c}(n) \bmod 2.$$

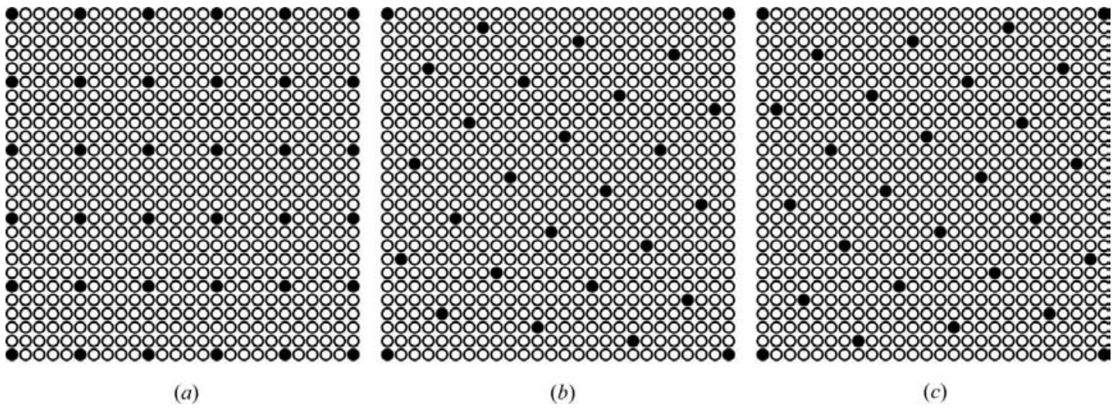

Figure 2
The three index-25 square sublattices of a $p4mm$ parent.

These arise from the various formulae for $p4$, $p2mm$ and $c2mm$. These functions only have odd values when there is a sublattice fixed by all the operations of $p4mm$, that is when F_{4mm} is nonzero. Since $f_E(n)$ is $\sigma_1(n)$, the sum-of-divisors function, this includes the well known result that $\sigma_1(n)$ is only odd if n is a square or twice a square.

(2) Since

$$f_E(n) + f_4(n) + f_{m_p}(n) + f_{m_c}(n) \equiv 0 \bmod 4$$

we have

$$\sigma_1(n) + \frac{r(n)}{4} + 2\sigma_0(n) \equiv 0 \bmod 4;\ \ 4 \nmid n$$

$$\sigma_1(n) + \frac{r(n)}{4} + 2\sigma_0(n) + 2\sigma_0(n/4) \equiv 0 \bmod 4;\ 4 \mid n.$$

Now $\sigma_0(n)$ is only odd if n is a complete square, so the third term of the left-hand side above is congruent to 0 mod 4 unless n is a square, as is the fourth term where it exists. Inserting these values gives

$$\sigma_1(n) + \frac{r(n)}{4} \equiv \begin{cases} 2 \bmod 4 & \text{if } n \text{ is an odd square,} \\ 0 \bmod 4 & \text{otherwise.} \end{cases}$$

(3) We note

$$f_E(n) \equiv f_6(n) \bmod 3.$$

This relationship, combined with $f_E(n) \equiv f_{m_c}(n) \bmod 2$, is enough to also ensure the requirement

$$f_E(n) + 2f_6(n) + 3f_{m_c}(n) \equiv 0 \bmod 6.$$

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