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On Colored Lattices and Lattice Preservation

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Dedicated to Dr David Harker on the occasion of his 75th birthday

Abstract

Two questions which have been independently studied (the distribution of colors in colored lattices and lattice preservation in derivative lattices) are in fact closely related. It is possible, for instance, to determine the distribution of colors in rows and nets by the lattice-preservation indices c_r and c_p as functions of row indices $[u_0,v_0,w_0]$ and net indices (h_0,k_0,l_0), respectively. A formula is also given for the number of classes of equivalent derivative lattices of a given index n.

1. Introduction

Recently two questions have been studied independently:

(1) The distribution of colors among the lattice points or nodes in the rows and the nets of a colored lattice L^c (Harker, 1978).

(2) The preservation of the lattice nodes by the rows and the nets of a derivative lattice (sublattice) L' of a lattice L (isomorphic subgroup of $P1$) (Billiet, 1979; Rolley-Le Coz & Billiet, 1980, 1981).

In fact these questions are closely related. Every derivative lattice can be identified with a colored lattice L^c and *vice versa*. We assign a single color to the nodes of the derivative lattice L'; the cosets of L', with respect to L, correspond to different colors. Every translation of the colored lattice L^c by a vector of L' leaves the color distribution in the lattice L^c unchanged, whereas a translation by an element of each of the cosets of L' corresponds to a certain color permutation, the same permutation for all members of a coset. The number n of distinct colors is equal to the index of L' in L. Conversely, the nodes of L^c with a single color define a derivative lattice L'.

In this paper we combine our efforts to clarify such misunderstood points as the distribution of colored nodes *as a function of the indices* of rows and nets. For definitions and terminology, the reader is referred to the previous papers.

2. Colored nodes and derivative lattices

Let L be a three-dimensional lattice and L' a sublattice of L of finite index. Primitive unit cells (a_0,b_0,c_0) of L and (a'_0,b'_0,c'_0) of L' may always be chosen in such a way that their vectors are related by the simple equations $a'_0=fa_0$, $b'_0=fgb_0$, $c'_0=fghc_0$. Here f, g and h are positive integers whose values are unique for a

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given sublattice L' of L, and $f^3g^2h = n$. The integers f, g and h do not define L' uniquely; two or more distinct sublattices may correspond to the same triple (f,g,h) [in theses cases, the choice of the primitive unit cell (a_0,b_0,c_0) will differ]. We define two sublattices of L to be equivalent if they correspond to the same triple.

Consider two parallel rows or nets, I and II, of a colored lattice L^c. Harker (1978) observed that 'either the colors in I are repeated on II in the same pattern or all the colors on II are different from those in I but form a pattern with the same abstract permutation group .... There are three possible types of colored lattices: (1) those in which *all rows* contain nodes of different colors – *i.e.* there are *no rows* of nodes of the same color; (2) those in which *there are rows* of nodes with the same color, but no nets of nodes colored all alike; and (3) those in which there *are nets* of nodes all colored the same.' The lattice L^c is type 1 if $f > 1$. L^c is type 2 if $f = 1, g > 1$. L^c is type 3 if $f = g = 1, h > 1$.

We can easily relate these observations to the study of the preservation of rows and nets by a derivative lattice (Rolley-Le Coz & Billiet, 1980, 1981; Rolley-Le Coz, 1982). Let $[u_0,v_0,w_0]$ be the row indices of a family ρ of rows of L with respect to (a_0,b_0,c_0); the greatest common divisor (GCD) of u_0, v_0 and w_0 is 1. We will denote the member of this family which contains the lattice-origin node by ρ_0. Then:

(α) Every c_r node of ρ_0 belongs to L', where $c_r = fgh/\mathrm{GCD}(gh,v_0h,w_0)$; c_r is called the preservation index of the family ρ.

(β) In the family ρ, one row out of n/c_r is preserved by L' in the same way as ρ_0, *i.e.* is a copy of ρ_0. The other rows contain no nodes of L'.

The preservation of a family π of nets of L by a derivative lattice L' obeys similar rules. Let (h_0,k_0,l_0) be the Miller indices of π with respect to (a_0,b_0,c_0); $\mathrm{GCD}(h_0,k_0,l_0) = 1$. Then:

(α′) One out of c_p nodes of the net π_0 containing the lattice-origin node is preserved by L', where $c_p = f^2g^2h/\mathrm{GCD}(h_0,k_0g,l_0gh)$; c_p is called the preservation index of the nets π.

(β′) One out of n/c_p nets π is preserved by L' in the same way as π_0; the other nets contain no nodes of L'.

In terms of the colored lattice L^c, (α) says that the row ρ_0 contains nodes of exactly c_p distinct colors, which repeat in cyclic order. Restating (β) in terms of L^c, we consider n/c_r successive rows. The first, ρ_0, contains nodes of c_r colors, the second contains nodes of c_r *other* colors, and so on. Similarly, (α′) says that π_0 contains nodes of c_p colors, and (β′) says that in a sequence of n/c_p successive nets, each net contains c_p different colors which are distinct from the colors of the other nets.

From (1) and (α) we see that if $f > 1$ then $c_r \geq f$ and $c_p \geq f^2g$. Thus $c_r > 1$ and $c_p > 1$. Therefore every row and every net contain more than one color. If $f = 1$ and $g > 1$, then $c_r \geq 1$ and $c_p > 1$. Thus in lattices of type 2, the nodes of the rows with indices of the form $u_0 = n_1$, $v_0 = n_2g$, $w_0 = n_3gh$, where n_1, n_2, n_3 are integers, have a single color (rows with other indices have nodes of more than one color). If $f = g = 1$, $h > 1$, then $c_r \geq 1$ and $c_p \geq 1$. In this case again the indices of certain rows and nets can be chosen so that $c_r = 1$ ($u_0 = n_1$, $v_0 = n_2g$, $w_0 = n_3gh$; n_1, n_2, n_3 are integers) and $c_p = 1$ ($h_0 = n_4h$, $k_0 = n_5h$, $l_0 = n_6$; n_4, n_5, n_6 are integers) and these rows and nets will contain nodes of a single color.

The concept of lattice preservation may be extended to rows and *hypernets* of lattices of *higher dimension d* (Rolley-Le Coz, 1981) and applied to the colored lattices connected with them. Let us consider in dimension d a lattice L and a derivative lattice L'. It is always possible to find a primitive unit cell $(a_1, a_2, \ldots, a_d)$ in L and a primitive unit $(a'_1, a'_2, \ldots, a'_d)$ in L' such that their vectors are simply related by equations $a'_1 = f_1a_1$, $a'_2 = f_1f_2a_2, \ldots, a'_d = f_1f_2\ldots f_da_d$, where $f_1, f_2, \ldots f_d$ are positive integers whose values are unique for a given family of equivalent sublattices of L; $f_1^d f_2^{d-1} \ldots f_d = n$. The preservation index of a row family $[u_1, u_2, \ldots, u_d]$ with $\mathrm{GCD}(u_1, u_2, \ldots, u_d) = 1$ is given by

$$c_r = (f_1f_2\ldots f_d)\,[\mathrm{GCD}(f_2f_3\ldots f_d, u_2f_3f_4\ldots f_d, \ldots, u_{d-1}f_d, u_d)]^{-1}$$

and the preservation index of a hypernet family $(h_1, h_2, \ldots, h_d)$ with $\mathrm{GCD}(h_1, h_2, \ldots, h_d) = 1$ is given by

$$c_p = n[f_1\mathrm{GCD}(h_1, h_2f_2, h_3f_2f_3, \ldots, h_df_2f_3\ldots f_d)]^{-1}.$$

Moreover, the lattice-preservation concept may be extended to *lattice varieties* whose dimension is intermediate between rows (dimension 1) and hypernets (dimension $d - 1$) (Rolley-Le Coz & Billiet, 1982).

3. The enumeration of derivative and colored lattices

The lattices L and L' can be regarded as space groups of type $P1$. Since $a'_0 = fa_0$, $b'_0 = fgb_0$ and $c'_0 = fghc_0$, it follows that L/L' is isomorphic to a direct product of three cyclic groups of orders f, fg and fgh. These numbers can be interpreted as the preservation indices of L by L' in the directions a_0, b_0, c_0 or, equivalently, as the number of colors in these rows. The number K of distinct classes of equivalent subgroups* L' of a given index is equal to the number of ways in which L/L' can be written as such a direct product. Senechal (1979) has shown that for the plane group $p1$ the definition of equivalence for derivative lattices given in this paper coincides with the definition of equivalence for color groups. Since her argument is valid in any dimension, K is the number of color groups of n colors associated with $P1$. In this section we calculate this number.

* The number of derivative lattices (not equivalence classes of lattices) has been found for any value of n (Billiet & Rolley-Le Coz, 1980).

We first show that the integers f, g and h determine the group $C_f \times C_{fg} \times C_{fgh}$. First we write fgh as a product of distinct primes $p_1^{e_{13}} p_2^{e_{23}} \ldots p_k^{e_{k3}}$, $e_{13} > 0$. Then fg can be written in the form $p_1^{e_{12}} p_2^{e_{22}} \ldots p_k^{e_{k2}}$, where $0 \leq e_{i2} \leq e_{i3}$. Finally, $f = p_1^{e_{11}} p_2^{e_{21}} \ldots p_k^{e_{k1}}$, and $0 \leq e_{i1} \leq e_{i2} \leq e_{i3}$. The order of the group $C_f \times C_{fg} \times C_{fgh}$ is then $f^3 g^2 h = n = p_1^{e_1} p_2^{e_2} \ldots p_k^{e_k}$, where $e_i = e_{i1} + e_{i2} + e_{i3}$.

If a and b are relatively prime then the direct product of the cyclic groups C_a and C_b of orders a and b is isomorphic to the cyclic group C_{ab} of order ab. Therefore

$$C_f = C_{p_1^{e_{11}}} \times C_{p_2^{e_{21}}} \times \ldots \times C_{p_k^{e_{k1}}},$$

$$C_{fg} = C_{p_1^{e_{12}}} \times C_{p_2^{e_{22}}} \times \ldots \times C_{p_k^{e_{k2}}},$$

and

$$C_{fgh} = C_{p_1^{e_{13}}} \times C_{p_2^{e_{23}}} \times \ldots \times C_{p_k^{e_{k3}}}.$$

Since the factors in a direct product commute, we have

$$\begin{aligned} C_f \times C_{fg} \times C_{fgh} = {} & (C_{p_1^{e_{11}}} \times C_{p_1^{e_{12}}} \times C_{p_1^{e_{13}}}) \\ & \times (C_{p_2^{e_{21}}} \times C_{p_2^{e_{22}}} \times C_{p_2^{e_{23}}}) \times \ldots \\ & \times (C_{p_k^{e_{k1}}} \times C_{p_k^{e_{k2}}} \times C_{p_k^{e_{k3}}}). \end{aligned}$$

The integers e_{ij} are called the invariants of the group. A basic theorem in group theory says that an Abelian group is completely characterized by its invariants, from which our assertion follows.

It follows that to enumerate the classes of equivalent derivative lattices of index n, we need to know the number of ways each e_i can be written as a sum of three non-negative integers e_{i1}, e_{i2}, e_{i3} with $0 \leq e_{i1} \leq e_{i2} \leq e_{i3} \leq e_i$. Let $n_3(e_i)$ represent this number. Then, since the partitions of the e_i are independent, any one can be combined with any other. Thus the number of ways of writing L/L' as a direct product of three cyclic groups is equal to the product $n_3(e_1) \ldots n_3(e_k)$.

This argument can easily be modified to hold for lattices in any dimension d.

Example: Let L be a two-dimensional lattice and L' a sublattice of index $n = 2^3 \times 5^4 \times 7 \times 11^2$. In dimension 2, $e_i = e_{i1} + e_{i2}$ and so $e_{i2} = e_i - e_{i1}$. Assuming $0 \leq e_{i1} \leq e_{i2} \leq e_i$, we obtain the following formula for $n_2(e_i)$:

$$n_2(e_i) = \begin{cases} (e_i + 1)/2 & \text{if } e_i \text{ is odd} \\ e_i/2 + 1 & \text{if } e_i \text{ is even.} \end{cases}$$

Thus $n_2(3) = 2$, $n_2(4) = 3$, $n_2(1) = 1$ and $n_2(2) = 2$. The product of these numbers is 12, so there are twelve classes of derivative lattices of index $n = 2^3 \times 5^4 \times 7 \times 11^2$.

Unfortunately there is no simple formula* for $n_d(e_i)$ except in the case $d = 2$. However, there is no difficulty in calculating $n_d(e_i)$ by hand if e^i is not too large (or by computer if it is).

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* *Note added in proof:* See, however, Kucab (1981).

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Bragg's Law in Higher Dimensions

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Abstract

Incommensurate modulated structures are no longer 'perfect' crystals in $\mathbb{E}^3$, where $\mathbb{E}^n$ is the n-dimensional affine Euclidian space; on the other hand they are crystals in $\mathbb{E}^4$, $\mathbb{E}^5$ or $\mathbb{E}^6$ whose cell is obtained from the experimental diffraction pattern in $\mathbb{E}^{*3}$. But Bragg's law is more general and it is shown that hyperplane incident waves are diffracted by sets of lattice hyperplanes of perfect crystals of $\mathbb{E}^n$.

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