Colored lattices

(generalized symmetry/Abelian groups/crystallography)

DAVID HARKER

Medical Foundation of Buffalo, Inc., 73 High Street, Buffalo, New York 14203

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ABSTRACT Combinations of translations and color permutations are derived that leave a periodic array of colored points—a colored lattice—apparently unchanged. It is found that there are three types of colored lattices: (1) those in which all rows and nets have more than one color, (2) those in which there are rows with only one color, and (3) those in which there are both rows and nets with only one color. The color permutation groups of colored lattices are all Abelian. The direct product of three independent cyclic subgroups is required by type 1, but only two are required by type 2; in type 3 the color permutation group consists of the n powers of a cyclic permutation of all n colors present—i.e., the group consists of a single cycle.

A lattice is a set of points, often called *nodes*, at vector distances from a chosen origin given by

$$\mathbf{L} = m\mathbf{a} + n\mathbf{b} + p\mathbf{c}, \quad [1]$$

where m , n , and p are any positive or negative integers, or zero, and $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ are three noncoplanar vectors. Such a set contains an infinitude of points. Any translational motion of this lattice by a distance and in a direction equal to one of the vectors $\mathbf{L}$ superimposes the points of the set upon their original positions, so that the new state of the set is indistinguishable from the old one. Thus the set of vectors $\mathbf{L}$ of Eq. 1 corresponds to a set of symmetry operations of the lattice. The addition of vectors is associative, and the zero vector $\mathbf{L} - \mathbf{L} = \mathbf{0}$ is a member of the set. These properties give the set of vectors $\mathbf{L}$ the nature of a mathematical group, the group “product” corresponding to addition and the negative of any vector $\mathbf{L}$ corresponding to its inverse. The unit member of the set is the zero vector $\mathbf{0}$.

The group $\{\mathbf{L}\}$ is Abelian, because $\mathbf{L} + \mathbf{L}' = \mathbf{L}' + \mathbf{L}$ always. Thus any subgroup of $\{\mathbf{L}\}$ is an invariant subgroup. Let a subgroup lattice $\{\mathbf{L}'\}$ of $\{\mathbf{L}\}$ be defined by

$$\mathbf{L}' = u\mathbf{a}' + v\mathbf{b}' + w\mathbf{c}', \quad [2]$$

with u , v , and w ranging over the integers, and

$$\begin{aligned} \mathbf{a}' &= t_{11}\mathbf{a} + t_{12}\mathbf{b} + t_{13}\mathbf{c} \\ \mathbf{b}' &= t_{21}\mathbf{a} + t_{22}\mathbf{b} + t_{23}\mathbf{c} \\ \mathbf{c}' &= t_{31}\mathbf{a} + t_{32}\mathbf{b} + t_{33}\mathbf{c} \end{aligned} \quad [3]$$

with the t_{jk} s arbitrary, but fixed, integers.

The ratio of the volumes of space per lattice point $V_{\mathbf{L}'} / V_{\mathbf{L}}$ is given by the magnitude of the determinant Δ of the matrix (t_{jk}) . The value of $|\Delta|$ is an integer and is the index of $\{\mathbf{L}'\}$ in $\{\mathbf{L}\}$ or the order of the factor group $\{\mathbf{L}/\mathbf{L}'\}$.

Suppose all the points defined by the vectors of the subgroup lattice $\{\mathbf{L}'\}$ have the same color (or other scalar property), and let the cosets of $\{\mathbf{L}'\}$ (each obtained by adding an $\mathbf{L}$ vector to all the $\mathbf{L}'$ vectors) correspond to different colors. (All the vectors $\mathbf{L}$ are encountered in this process.) Then the number of dif-

ferent colors will be $|\Delta|$, because there are $|\Delta|$ points of the set $\{\mathbf{L}\}$ for each point of the set $\{\mathbf{L}'\}$. Every translation of the colored lattice $\mathbf{L}^c$ by a vector of the set $\{\mathbf{L}'\}$ leaves the color distribution on the lattice $\mathbf{L}^c$ apparently unchanged—i.e., corresponds to the nonpermutation $(-)$ of the colors—whereas a translation by a member of each of the several cosets of $\{\mathbf{L}'\}$ corresponds to a certain color permutation, the same permutation for all members of a coset. This treatment is based on the work of van der Waerden and Burckhardt (1).

The factor group $\{\mathbf{L}/\mathbf{L}'\}$ with the order $|\Delta|$ is isomorphic to the permutation group P_n of the n colors ($n = |\Delta|$) used in constructing the colored translation operators which leave the colored lattice $\mathbf{L}^c$ invariant. (Strictly, this P_n is a subgroup of the complete permutation group of n colors, because the latter has $n!$ members, whereas P_n consists of only n members.) Because lattice translations are vectors and vector sums are commutative, the members of the permutation group P_n must also commute; P_n is thus Abelian.

Eqs. 1, 2, and 3 are all written for three-dimensional lattices, but two-dimensional lattices, or nets, and one-dimensional lattices, or rows, can be treated by simple specializations of these equations.

The three-dimensional colored lattices

A three-dimensional colored lattice* can be thought of as a stack of geometrically congruent, parallel colored rows or nets. Each of these rows or nets has a colored translation group of its own. Consider two parallel rows or nets I and II of the stack. Let $\{\mathbf{M}\}$ and $\{\mathbf{M}'\}$ be, respectively, the subgroups of $\{\mathbf{L}\}$ and $\{\mathbf{L}'\}$ which consist of all their lattice translations parallel to rows or nets I and II. The color permutation groups of I and II are isomorphic to the quotient group (factor group) $\{\mathbf{M}/\mathbf{M}'\}$ and consequently to each other. Therefore, 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-translation group.

This last statement can be proved as follows: (i) If a color, say 1, on I also occurs on II, then color 2 must occur at the same vector distance from color 1 in II as it does in I. And so on, for every color in II, thus making it color-congruent to I. (ii) If a color, say k , not on I, occurs on II, then there is a colored lattice translation that brings I into coincidence with II, and changes a color, say 2, on I into the color k on II. And there must be a different color on II corresponding to each different color on I, and not even one of these can be the same as a color on I because of i above, q.e.d.

The argument in the preceding paragraph proves that the number of colors, n , in a colored lattice either is the same as the number of colors in a single net or row of the lattice or is some integral multiple of it. If the value of n is prime, the nets and rows of the lattice contain either all the n colors or only one

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Abbreviation: PUC, primitive unit cell.

* Colored lattices are mentioned in ref. 2. This book also contains an extensive table of references to colored symmetry.

color. Therefore, a lattice with a prime number of colors can always be treated as a stack of nets each with a single color, and the colors must follow each other up the stack in a repetitive sequence n colors long. The color permutations are, in this case, all powers of a cycle of length n , and the permutation group has the structure C_n .

Any number of colors, n , can be used to form a colored lattice by stacking one-colored nets one above the other in a sequence of n colors that repeats with the period n . However, if n is not prime, nets and rows with colored symmetry involving an aliquot part of the number of different colors present are also possible. Such colored lattices can involve permutation groups with structures other than C_n , but only if a noncyclic Abelian group of order n exists.

A general theoretical framework for the translational symmetry properties of colored lattices

In general, an Abelian group P can be expressed as the direct product of a number of cyclic groups; thus: $P = C_j \times C_k \times C_l \times \dots \times C_t$. The order of P is $n = jkl \dots t$. If a pair of cycles with coprime order occurs in this product—e.g., C_p and C_q with $(p, q) = 1$ —then their product $C_p \times C_q$ can be reformulated as a single cycle C_r with the order $r = pq$. By combining pairs of cycles in this way, the number of cycles in P can be reduced until either (i) the orders of all pairs of cycles in P have a common factor, or (ii) P is reduced to a single cycle. Examine case i: Take the members of one of these pairs to be C_l and C_m with $l = fl'$ and $m = fm'$. Then, it is known that $C_l \times C_m$ can be reformulated as $C_f \times C_{f'l'm'}$ —i.e., as the direct product of two cycles, one of which has the order f , while the other has an order that is a multiple of f . When all the pairs of cycles in P have been reformulated in this way and the resulting product is written with the orders of the cycles increasing from left to right, it follows that $P = C_f \times C_{fg} \times C_{fgh} \times \dots \times C_{fgh \dots pq}$ and has the order $f^t g^{t-1} h^{t-2} \dots q$, where t is the final number of cycles. This will be called the *stable* form of P . These results are derived in ref. 3.

The set of colored symmetry operations S of a colored lattice L^c is a homomorphic mapping of lattice translation group T onto color permutation group P . The abstract structure of the group $\{P\}$ is Abelian, and is, in general, the direct product of three cyclic subgroups. Thus, we can write: $S = (ma + nb + pc) [P_a^m \times P_b^n \times P_c^p]$. Here, m , n , and p are any integers; a , b , and c are the vectors defining a primitive unit cell (PUC) of L ; and P_a , P_b , and P_c are the color permutations connected with the translations a , b , and c , respectively. The complete permutation $P = P_a^m \times P_b^n \times P_c^p$ is combined with $T = ma + nb + pc$ to form the colored symmetry operation S . The order of the group $\{P\}$ is $|\Delta|$. $\{P\}$ is isomorphic to $\{L/L'\}$.

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 all 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 color permutation groups in the colored symmetry groups of these three types of colored lattices have abstract structures that are all Abelian. However, the

“stable” forms differ:—type 1 contains three independent cyclic subgroups, type 2 contains two independent cyclic subgroups, and type 3 contains only a single cycle.

Table 1 sets forth the characteristics of the three general types of colored lattices.

Eqs. 3 relate the vectors a' , b' , c' defining a PUC of the one-colored subgroup lattice L' to the vectors a , b , c defining a PUC in the color-blind lattice L . Both of these vector triples can be chosen in a number of ways, and the question arises, “How are the numbers t_{jk} affected by changing from one PUC to another in L or L' ?”

First consider L . The vectors $ma + nb$, with m, n any integers, define a net plane through the origin. The vector c (which is not in this plane) terminates at a point in the next parallel net plane. The unit cell defined by a , b , and c is primitive no matter which point in the parallel net is chosen to terminate c —i.e., c can be replaced by $\gamma = c + pa + qb$, where p and q are any integers, and the cell defined by a , b , and γ will still be primitive.

In Eqs. 3 substitute c by $\gamma - pa - qb$, and obtain:

$$\begin{aligned} a' &= (t_{11} - pt_{13})a + (t_{12} - qt_{13})b + t_{13}\gamma \\ b' &= (t_{21} - pt_{23})a + (t_{22} - qt_{23})b + t_{23}\gamma \\ c' &= (t_{31} - pt_{33})a + (t_{32} - qt_{33})b + t_{33}\gamma \end{aligned} \quad [3']$$

That is to say: the lattice L' is described in terms of the same triple a' , b' , c' if γ replaces c , $t_{j1} - pt_{j3}$ replaces t_{j1} , and $t_{j2} - qt_{j3}$ replaces t_{j2} —i.e., integral multiples of the numbers in any column of (t_{jk}) can be added to, or subtracted from, the corresponding numbers in any other column in (t_{jk}) without changing the relationship between L' and L (because the choice of the net plane $ma + nb$ was arbitrary).

A similar treatment, but now in the L' lattice, leads to the conclusion that integral multiples of the t_{jks} in any row can be added to, or subtracted from, the t_{jks} in any other row of (t_{jk}) without fundamentally changing the meaning of Eqs. 3. (It is well known that such operations as those described in this and the preceding paragraph leave the value of the determinant $|t_{jk}|$ unchanged.)

We now proceed to discover whether the lattice is of type 1, 2, or 3 by examining the properties of the matrix (t_{jk}) . First, when all the t_{jks} have a common factor greater than unity, the lattice is of type 1; this will be proved below. Second, when the value of the determinant $\Delta = |t_{jk}|$ —i.e., the number of colors n —is not divisible by a perfect square larger than unity, then the lattice is of type 3. Third, when the value of Δ is divisible by a perfect square larger than unity and there are two coprime elements in (t_{jk}) , then the lattice may be of either type 2 or 3; it will be shown below how to find out which it is.

We first review a few properties of numbers. Suppose we are dealing with a pair of coprime numbers, f and g . Let us add a multiple of one, say f , to the other, thus obtaining a new pair f and $fm + g$. The numbers in this new pair are still coprime, because a factor of f is a factor of fm , but not of g , since f and g are coprime.

Now take another pair of numbers pf and pg with a common

Table 1. Characteristics of colored lattices

Type of colored lattice	Contains one-colored rows	Contains one-colored nets	Number of colors	Stable form of permutation group	Order n
1	No	No	Divisible by a cube	$C_f \times C_{fg} \times C_{fgh}$	$f^3 g^2 h$
2	Yes	No	Divisible by a square	$C_g \times C_{gh}$	$g^2 h$
3	Yes	Yes	Arbitrary	C_n	n

factor p . The addition of a multiple of one to the other results in a new number that is also divisible by p , because $mpf + pg = p(mg + g) = ph$.

Thus, when there is, in the matrix (t_{jk}) , a row composed of coprime integers, adding or subtracting multiples of columns to, or from, other columns cannot introduce a common factor into the given row nor remove from it a common factor already present, even though the numbers in the row have been changed into others during the process. (The same statements apply when the words "row" and "column" in this paragraph are interchanged.)

It is well known that, in the expression $\alpha p + \beta q = t$, where p and q are a fixed pair of coprime integers, the value of t may be made equal to any desired integer by giving appropriate integral values to α and β . By using this property of coprime integers and adding to columns multiples of other columns, we can change the three t_{jk} s in any coprime row into a figure 1 (i.e., unit) in any one column and zeros in the other two columns. Thereafter the two other t_{jk} s in the column containing the unit can be changed to zeros by the addition or subtraction of multiples of the unit in the originally given row. This process corresponds to our choosing new unit cells in the L and L' lattices so that they have one edge in common.

Similarly, if the three t_{jk} s in a row were to have a highest common factor f , that row can be changed into one containing two zeros and an f by an analogous process. This means that axes can be chosen in the L and L' lattice so that the PUC in L' has an edge that is f times an edge of the PUC of L .

We now "diagonalize" the (t_{jk}) matrix for a colored lattice of type 1. We then show that types 2 and 3 are special cases of type 1.

Assume all t_{jk} s to have a highest common factor f . Then, by adding and subtracting multiples of columns and rows of the matrix from and to, respectively, other columns and rows, produce a new matrix containing the factor f in the t_{11} position and zeros in the t_{12} and t_{13} positions. Then make t_{21} and t_{31} equal to zero by continuing this process. This reformulation of the matrix (t_{jk}) can always be carried out. (See ref. 4.)

Now consider the four-member matrix consisting of the elements t_{22} , t_{23} , t_{32} , and t_{33} . In the general case these four matrix elements have a highest common factor fg . Proceed, as before, to obtain a new four-member matrix with its two off-diagonal elements t_{23} and t_{32} equal to zero; its diagonal elements t_{22} and t_{33} will then be equal to fg and fgh , respectively.

This "diagonalization" shows that axes can be chosen in the L and L' lattices, so that L' can be related to L by the equations: $a' = fa$, $b' = fgb$, $c' = fghc$. The number of colors $n = f^3g^2h$; it is the magnitude of the determinant $|t_{jk}|$. The lattice is type 1 in the general case, where f , g , and h are all greater than unity, because every vector in L' is at least f times a vector in L .

The permutation of the n colors accompanying a translation by a in the colored L^c lattice is a product of n/f cyclic color permutations, each of f colors. This permutation P_a has the period f and generates a group with the abstract structure C_f . Similarly, a translation by b carries with it a color-permutation P_b consisting of the product of n/fg cycles, each of fg colors; its period is fg and it generates a group with the abstract structure C_{fg} . Finally, a translation by c of the colored L^c lattice is joined to a product of n/fgh color permutations, each of period fgh , and it generates a permutation group P_c with the abstract structure C_{fgh} . The complete Abelian permutation group P of the colored L^c lattice thus has the abstract structure $C_f \times C_{fg} \times C_{fgh}$, and is in "stable" form.

It usually happens that the number of colors n is not divisible by a perfect cube or a perfect square (larger than unity), and the lattice is consequently of type 3. For all such values of n the only possible structure of the permutation group is C_n (because $f = g = 1$), and the permutations accompanying translations of the colored L^c lattice are all powers of a single cyclic permutation—e.g., $(1\ 2\ 3\ \dots\ n)$. In these cases it is usually convenient to choose the PUCs in L and in L' so that $a' = a$, $b' = b$, and $c' = nc$. However, symmetry considerations may make other choices of the PUCs more suitable.

When n is divisible by a perfect cube or a perfect square, but

Table 2. Abstract structures of colored translation groups for various numbers of colors

No. of colors	Structures	No. of colors	Structures
1	C_1	25	$C_{25}, C_5 \times C_5$
2	C_2	26	C_{26}
3	C_3	27	$C_{27}, C_9 \times C_3, C_3 \times C_3 \times C_3$
4	$C_4, C_2 \times C_2$	28	$C_{28}, C_{14} \times C_2$
5	C_5	29	C_{29}
6	C_6	30	C_{30}
7	C_7	31	C_{31}
8	$C_8, C_4 \times C_2, C_2 \times C_2 \times C_2$	32	$C_{32}, C_{16} \times C_2, C_8 \times C_4, C_8 \times C_2 \times C_2, C_4 \times C_4 \times C_2$
9	$C_9, C_3 \times C_3$	33	C_{33}
10	C_{10}	34	C_{34}
11	C_{11}	35	C_{35}
12	$C_{12}, C_6 \times C_2$	36	$C_{36}, C_{18} \times C_2, C_{12} \times C_3, C_6 \times C_6$
13	C_{13}	37	C_{37}
14	C_{14}	38	C_{38}
15	C_{15}	39	C_{39}
16	$C_{16}, C_8 \times C_2, C_4 \times C_4, C_4 \times C_2 \times C_2$	40	$C_{40}, C_{20} \times C_2, C_{10} \times C_2 \times C_2$
17	C_{17}	41	C_{41}
18	$C_{18}, C_6 \times C_3$	42	C_{42}
19	C_{19}	43	C_{43}
20	$C_{20}, C_{10} \times C_2$	44	$C_{44}, C_{22} \times C_2$
21	C_{21}	45	$C_{45}, C_{15} \times C_3$
22	C_{22}	46	C_{46}
23	C_{23}	47	C_{47}
24	$C_{24}, C_{12} \times C_2, C_6 \times C_2 \times C_2$	48	$C_{48}, C_{24} \times C_2, C_{12} \times C_4, C_{12} \times C_2 \times C_2$

(t_{jk}) contains two elements that are coprime integers, then $f = 1$, and the stable form of the color-permutation group cannot consist of more than two cycles—e.g., $C_g \times C_{gh}$, with $g^2h = n$. In this case, it is necessary to carry through the first stage of diagonalization of the matrix (t_{jk}) in order to find out whether the resulting four-member matrix consists of elements with a common factor g greater than unity. If so, two cycles are present, and the lattice is of type 2; if not, the permutation group is C_n , and the lattice is of type 3.

An interesting example is the case in which L is face-centered cubic and L' consists of the cubic lattice without the centerings. Using the primitive rhombohedral cell for L , the matrix (t_{jk}) takes the form $(\bar{1}\bar{1}1/1\bar{1}1/1\bar{1}\bar{1})$. Here $|\Delta| = n = 4$. Diagonalization, as described above, results in $(100/020/002)$, which shows the permutation group to have the structure $C_2 \times C_2$, and the lattice L^c to be of type 2.

Table 2 lists the possible structures of the permutation groups connected with translation groups for various useful numbers of colors in colored lattices.

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