

# Theory of color symmetry for periodic and quasiperiodic crystals

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The author presents a theory of color symmetry applicable to the description and classification of periodic as well as quasiperiodic colored crystals. This theory is an extension to multicomponent fields of the Fourier-space approach of Rokhsar, Wright, and Mermin. It is based on the notion of indistinguishability and a generalization of the traditional concepts of color point group and color space group. The theory is applied toward (I) the classification of all black and white space-group types on standard axial quasicrystals in two and three dimensions; (II) the classification of all black and white space-group types in the icosahedral system; (III) the determination of the possible numbers of colors in a standard two-dimensional  $N$ -fold symmetric color field whose components are all indistinguishable; and (IV) the classification of two-dimensional decagonal and pentagonal  $n$ -color space-group types, explicitly listed for  $n \leq 25$ . [S0034-6861(97)00604-1]

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## I. INTRODUCTION

We shall describe here a theory of color symmetry that extends the ideas of traditional theories of color symmetry for periodic crystals to the broader category of quasiperiodic crystals. The basic notion is that of associating a certain attribute, or color, to each of the crystal sites. The different colors may correspond, for example, to different chemical species, or the different orientations of a magnetic moment, or may represent an actual coloring of a periodic or quasiperiodic drawing. The colored crystal is said to have color symmetry if rotations (and, in the special case of periodic crystals, translations) that are symmetry operations of the uncolored crystal may be combined with global permutations of the colors to become symmetry operations of the colored crystal.

Before turning to the description of our theory and the main body of this work we first introduce the basic terminology used in dealing with quasiperiodic crystals and clarify exactly what we mean when we say that a certain rotation is a symmetry of a crystal. We also include in this Introduction a short account of the existing work on the color symmetry of quasiperiodic crystals.

### A. Quasiperiodic crystals

The International Union of Crystallography (1992) defines a *crystal* to be “...any solid having an essentially discrete diffraction diagram.” We shall be slightly more specific and consider only *quasiperiodic crystals*. These

are crystals whose diffraction diagrams are “essentially discrete” by virtue of having density functions with well defined Fourier expansions

$$\rho(\mathbf{r}) = \sum_{\mathbf{k} \in L} \rho(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} \quad (1)$$

that require at most a countable infinity of plane waves. In a real diffraction experiment only a finite number of Bragg peaks will be observed.

The set  $L$ , consisting of all integral linear combinations of the wave vectors appearing in the Fourier expansion in Eq. (1), is called the *lattice* or the *Fourier module* of the crystal. In all experimentally observed crystals the lattice may be expressed as the set of all integral linear combinations of a finite number of wave vectors. The minimum number  $D$  of vectors needed to generate the lattice in this way is called its *rank* or its indexing dimension. A quasiperiodic crystal is periodic if and only if the rank of its lattice is equal to the physical dimension  $d$ . Only then is the lattice a conventional “reciprocal lattice” related in the familiar way to a lattice of real-space translations under which the periodic crystal is invariant (see, for example Ashcroft and Mermin, 1976, Chap. 5). The set of (proper or improper) rotations,<sup>1</sup> which when applied to the origin of Fourier space merely permute the wave vectors of the lattice, forms a group called the *lattice point group*  $G_L$  (also called the holohedry).

### B. Restoring the notion of symmetry

The traditional theory of crystal symmetry describes the symmetry of a crystal by its space group, the set of rigid motions in  $d$ -dimensional space—combinations of translations and rotations—that leave the crystal invariant. Such a description is not valid for quasiperiodic crystals, not only because there are no longer any translations that leave the crystal invariant, but also because there are, in general, no rotations that leave the crystal invariant.

Two approaches have been taken to extending the theory of space groups to quasiperiodic crystals. The “superspace approach” of de Wolff, Janner, and Janssen (de Wolff, Janssen, and Janner, 1981; Yamamoto *et al.*, 1985; Janssen *et al.*, 1992) treats the quasiperiodic crystal as a  $d$ -dimensional slice of a structure periodic in a higher-dimensional “superspace.” The symmetry of the quasiperiodic crystal is then given by the high-dimensional space group describing the set of rigid motions in superspace that leave invariant the high-dimensional structure. The “Fourier-space approach” of Rokhsar, Wright, and Mermin (1988a; 1988b), which we shall follow here, treats the quasiperiodic crystal directly in  $d$ -dimensional space by introducing the notion of indistinguishability and redefining the concept of point-group symmetry.

<sup>1</sup>Throughout the paper the term “rotation” refers to proper as well as improper rotations.

The key to this redefinition is the observation that certain rotations (proper or improper), when applied to a quasiperiodic crystal, take it into one that looks very much like the unrotated crystal. This is because the two crystals are *indistinguishable*—they contain the same spatial distribution of bounded structures of arbitrary size.<sup>2</sup> One finds that any bounded region in the unrotated crystal is reproduced some distance away in the rotated crystal, but there is, in general, no single translation that brings the whole crystals into perfect coincidence. This weaker notion of symmetry is captured by defining a crystal to have the symmetry of a certain rotation if that rotation leaves invariant all spatially averaged density autocorrelation functions,

$$C^{(n)}(\mathbf{r}_1, \dots, \mathbf{r}_n) = \lim_{V \rightarrow \infty} \frac{1}{V} \int d\mathbf{r} \rho(\mathbf{r}_1 - \mathbf{r}) \cdots \rho(\mathbf{r}_n - \mathbf{r}). \quad (2)$$

In the case of periodic crystals this reduces to the familiar requirement that the rotated and the unrotated crystals differ at most by a translation.

The Fourier-space approach receives its name from the fact that indistinguishability is more easily expressed in Fourier space in terms of the density Fourier coefficients  $\rho(\mathbf{k})$ . It can be shown that two densities  $\rho$  and  $\rho'$  are indistinguishable if their Fourier coefficients are related by

$$\rho'(\mathbf{k}) = e^{2\pi i \chi(\mathbf{k})} \rho(\mathbf{k}), \quad (3)$$

where  $\chi$ , called a *gauge function*, is linear modulo an integer over the lattice  $L$  of wave vectors. By this we simply mean that  $\chi(\mathbf{k}_1 + \mathbf{k}_2) \equiv \chi(\mathbf{k}_1) + \chi(\mathbf{k}_2)$  whenever  $\mathbf{k}_1$  and  $\mathbf{k}_2$  are in  $L$ , where “ $\equiv$ ” denotes equality to within an additive integer. With such a simple expression at hand one can define the *point group*  $G$  of a scalar quasiperiodic density  $\rho$  to be the set of operations  $g$  from  $O(3)$  satisfying

$$\rho(g\mathbf{k}) = e^{2\pi i \Phi_g(\mathbf{k})} \rho(\mathbf{k}), \quad (4)$$

where the gauge functions  $\Phi_g(\mathbf{k})$ , one for each element of the point group, are called *phase functions*. It should be clear from the point-group condition (4) that  $G$  is necessarily a subgroup of the lattice point group  $G_L$ . The point group  $G$  along with its set of phase functions constitutes the generalization of the concept of a space group for quasiperiodic crystals.

The Fourier-space approach has been applied successfully to the classification of a large variety of periodic and quasiperiodic crystals (see, for example, the references cited by Lifshitz, 1996a). Although this paper is intended to be self-contained, the reader who is unfamiliar with the approach might benefit from the detailed review by Mermin (1992) or at least the introduction by Lifshitz (1996a) to the Fourier-space approach as it is used in the context of standard (uncolored) space groups.

<sup>2</sup>In the language of tiling theory, two tilings that possess this property are said to be “locally isomorphic.”

We shall extend the notion of indistinguishability to colored crystals by requiring that any rotation that is to be a symmetry operation of a colored crystal leave it indistinguishable to within a global permutation of the colors. This will provide the basis for a redefinition of the concept of a color point group and the starting point of our theory.

### C. Existing work on the color symmetry of quasiperiodic crystals

The problem of color symmetry has been studied extensively in the context of periodic crystals. Applications range from the symmetry analysis of the periodic drawings of M. C. Escher (Macgillavry, 1965) to the description of order-disorder phase transitions and the structural analysis of magnetic crystals. We refer the reader to the review by Schwarzenberger (1984), which contains an extensive bibliography on the subject, and also to the relevant chapters of the book by Opechowski (1986).

Only a few authors to date have considered the classification of color groups in the context of quasiperiodic crystals. Niizeki (1990a; 1990b) has classified in superspace the icosahedral black and white Bravais classes and the black and white Bravais classes of lattices with axial point groups of 5-, 8-, 10-, and 12-fold symmetry. He used his results to discuss the possibility of order-disorder transformations in which, in the ordered phase, two chemical species are arranged according to the black and white coloring of the structure. We shall express the notion of colored lattices in the language of our theory and in Sec. V extend Niizeki’s results to standard axial lattices of arbitrary rotational symmetry. Sheng (1994) and Sheng and Elser (1994) have enumerated some of the icosahedral black and white space-group types for the purpose of constructing quasiperiodic minimal surfaces. The minimal surface, like a soap film, describes the state of equilibrium of the interface between two fluid phases, associated with the two colors, and is constructed by minimizing an appropriate free-energy functional. Elser (1995) has used a similar approach to construct equilibrium configurations of Coulomb charges in two dimensions, which have the symmetry of a four-color octagonal space group. Lifshitz and Mermin (1995) have given an ad hoc classification of the two-color and five-color decagonal and pentagonal space groups in two dimensions. In Sec. VII we shall give a general solution to the classification of decagonal and pentagonal  $n$ -color space groups, listing them explicitly for  $n \leq 25$ .

The issue of colored quasiperiodic tilings has been addressed by even fewer authors. Li, Dubois, and Kuo (1994) introduced a black and white Penrose tiling along with its inflation rules (shown in Fig. 1) and used it for structural analysis of the alternating layers in decagonal quasicrystals. Lück (1987; 1995) has introduced a five-colored Penrose tiling (shown in Fig. 3) and used it for the analysis of screw dislocations in decagonal quasicrystals. Scheffer and Lück (1996) have produced additional

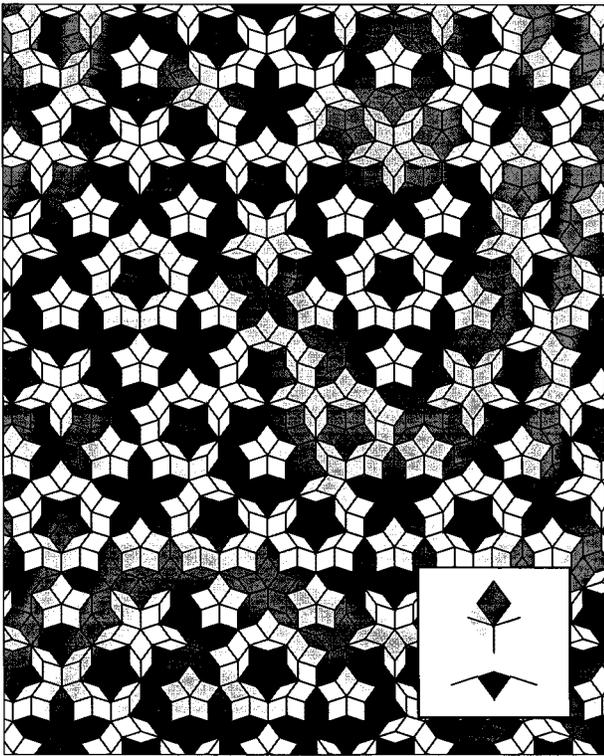


FIG. 1. The two-color Penrose tiling of Li, Dubois, and Kuo (1994). Using the notation of Sec. V, we find that the black and white space group of this tiling is  $10'm'm$ . A tenfold rotation and a horizontal mirror reflection both require the exchange of black and white to leave the tiling indistinguishable, whereas a vertical mirror reflection does not. The tiling is created using a standard inflation procedure and associating colors with the segments of the inflated tiles. The coloring of the inflated white tiles is shown in the inset, the coloring of the inflated black tiles is reversed.

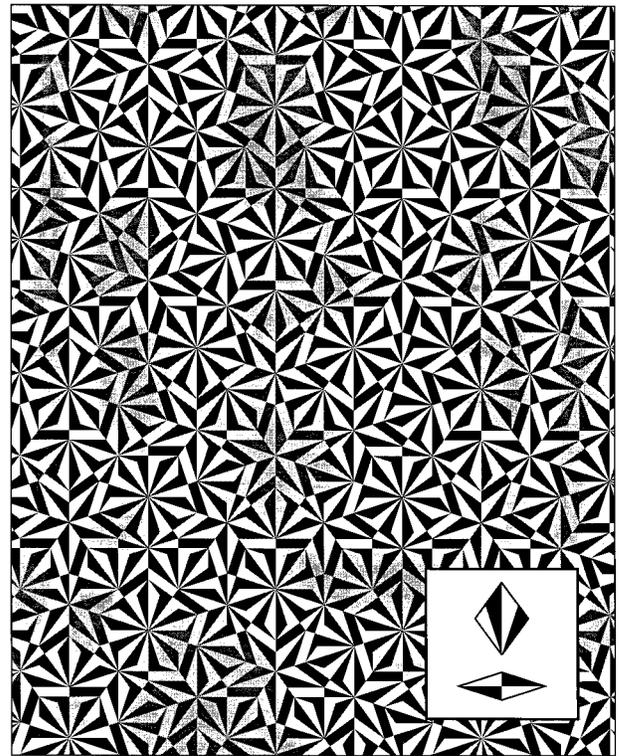


FIG. 2. A two-color Penrose tiling with black and white space group  $10m'm'$ . Both a horizontal mirror reflection and a vertical mirror reflection require the exchange of black and white to leave the tiling indistinguishable, whereas a tenfold rotation does not. The inset shows the scheme by which the Penrose tiles are colored to produce this two-color tiling. The orientation of the black and white triangles within the thick rhombus is determined according to the matching rules (which are not indicated in the figure).

decagonal tilings using an ad hoc method of Amman grids, all with the same five-color space-group type. Additional colored tilings, included in this paper (Figs. 2 and 4), have also been created ad hoc. We shall defer to a subsequent publication the question of general methods for generating quasiperiodic tilings with prescribed color symmetry.

Moody and Patera (1994) have considered the symmetric coloring of quasicrystals from an algebraic point of view. Baake (1997) has used algebraic methods to count the number of invariant sublattices of a given index in a given parent lattice. We shall see later that this question is related to the enumeration of color space groups. In Sec. VI we shall address a similar counting problem on standard two-dimensional axial lattices using a geometric approach.

#### D. Organization of the paper

In Sec. II we extend the notion of indistinguishability to colored crystals and introduce the concepts of “color

point group” and “color space group,” used in the description of such crystals. In Sec. III we establish the symmetry classification scheme for colored crystals, which is an organization of lattices, color point groups, and color space groups into equivalence classes. In Sec. IV we delve into the group-theoretic details that underly our approach. In Sec. V we apply our theory to the simplest case—black and white symmetry—and enumerate all black and white space-group types on standard axial lattices in two and three dimensions, as well as all the black and white space-group types in the icosahedral system. As a second application, we discuss in Sec. VI the question of invariant sublattices of standard two-dimensional axial lattices. We conclude with a third application in Sec. VII, where we give a general solution to the classification of two-dimensional decagonal and pentagonal  $n$ -color space groups, listing them explicitly for  $n \leq 25$ . In the appendix we prove—in a context more general than just color symmetry—that the statement of indistinguishability in Fourier space, used throughout the paper, is indeed equivalent to the real-space definition of this notion.

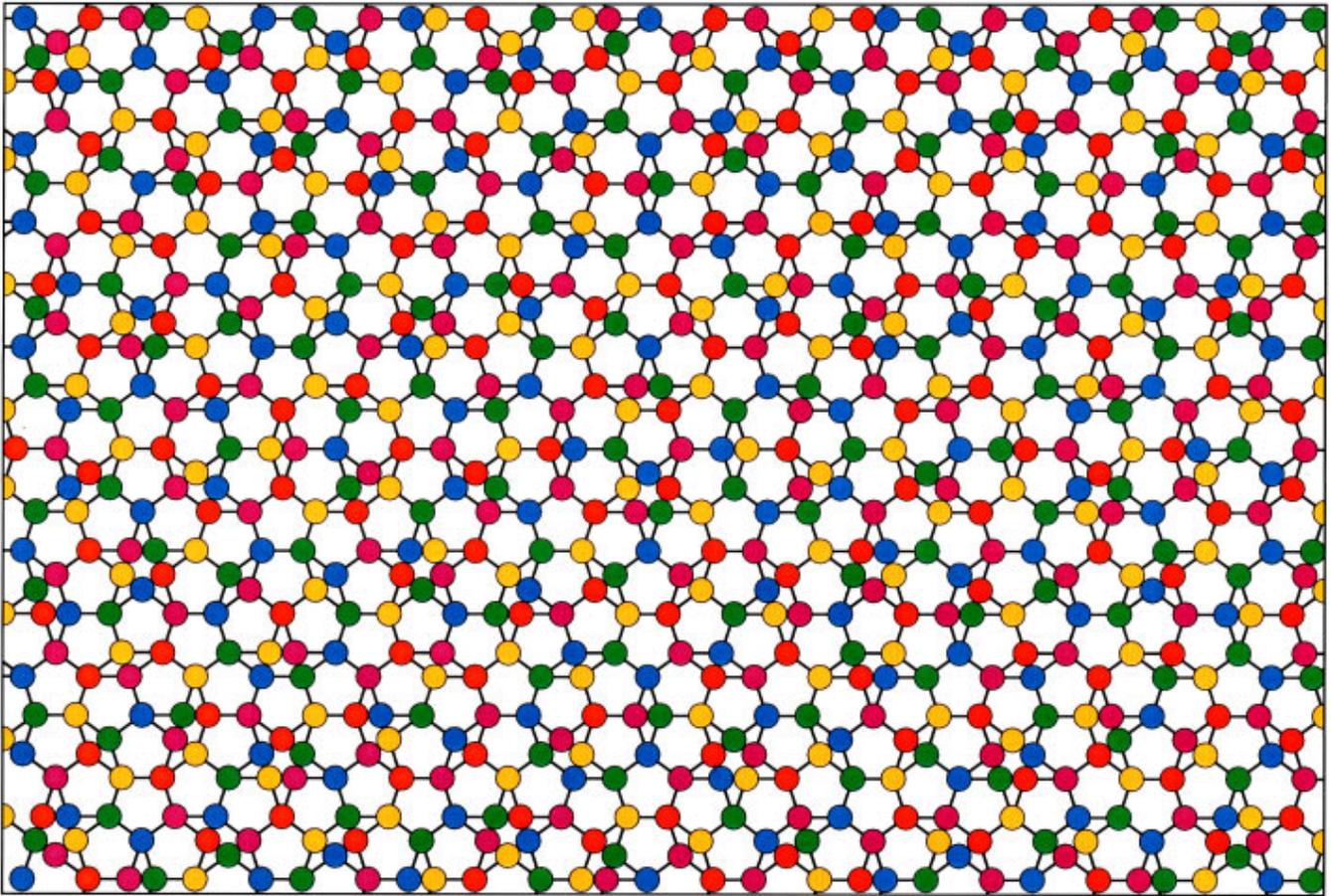


FIG. 3. (Color) The five-color Penrose tiling used by Lück (1995) for the analysis of screw dislocations in decagonal quasicrystals. All five colors belong to a single indistinguishability class. The lattice color group  $\Gamma_c$  is a cyclic group of order 5 ( $\cong Z_5$ ), generated by the permutation  $\gamma = (C^1 C^2 C^3 C^4 C^5)$ . The color point group is listed as number 5.b.1 in Table XIII. It is generated by  $(e, \gamma)$ ,  $(r_{10}, \delta)$ , and  $(m_1, \epsilon)$  and denoted by  $(10mm, 10mm, 10mm, 5m1 | Z_5)$  according to the notation of Sec. VII, which is summarized in the caption of Table XIII. The color space-group type is given by the phase function  $\Phi_c^\gamma$ , which has the value 1/5 on the lattice-generating vectors, and the two phase functions  $\Phi_{r_{10}}^\delta$  and  $\Phi_{m_1}^\epsilon$ , which are zero everywhere.

## II. DESCRIBING THE SYMMETRY WITH A COLOR SPACE GROUP

### A. The color field

We represent the colored quasiperiodic crystal by an  $n$ -component vector field  $\vec{\rho}(\mathbf{r})$  whose  $i$ th component  $\rho_i(\mathbf{r})$  gives the density of points with color  $c_i$ . We always assume that the number of colors  $n$  is finite and that no two components of  $\vec{\rho}$  are identical scalar functions<sup>3</sup> of  $\mathbf{r}$ . Color permutations that are combined with spatial rotations to leave the colored crystal indistinguishable are represented as permutation matrices acting on the components of the color field. We should note that  $\vec{\rho}(\mathbf{r})$  is not endowed with the full transformation properties of a vector and is only acted upon by

these permutation matrices. We need one further reasonable restriction on the color field  $\vec{\rho}(\mathbf{r})$  so that we come up with a sensible theory of color symmetry. We follow the widely accepted requirement (Senechal, 1975, 1979; Schwarzenberger, 1984) that any two patterns of different colors are related at least by one symmetry operation of the crystal. This means that for any two components of the color field there is at least one permutation that takes one into the other.

Because the colored crystal is quasiperiodic we can expand the color field  $\vec{\rho}$  as a sum of countably many plane waves with vector coefficients

$$\vec{\rho}(\mathbf{r}) = \sum_{\mathbf{k} \in L} \vec{\rho}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}}. \quad (5)$$

The *lattice*  $L$  is now defined as the set of all integral linear combinations of wave vectors  $\mathbf{k}$  for which at least one component of  $\vec{\rho}(\mathbf{k})$  is nonzero. The total density of the crystal  $\rho_0(\mathbf{r})$ , called the *color-blind density* (borrowing from Harker, 1978b), is equal to the sum of all the

<sup>3</sup>The latter assumption might seem obvious, but in the early days of research on black and white groups one would allow the black and the white to overlap exactly, creating structures whose symmetry was described using so called “gray groups.” We exclude such possibilities.

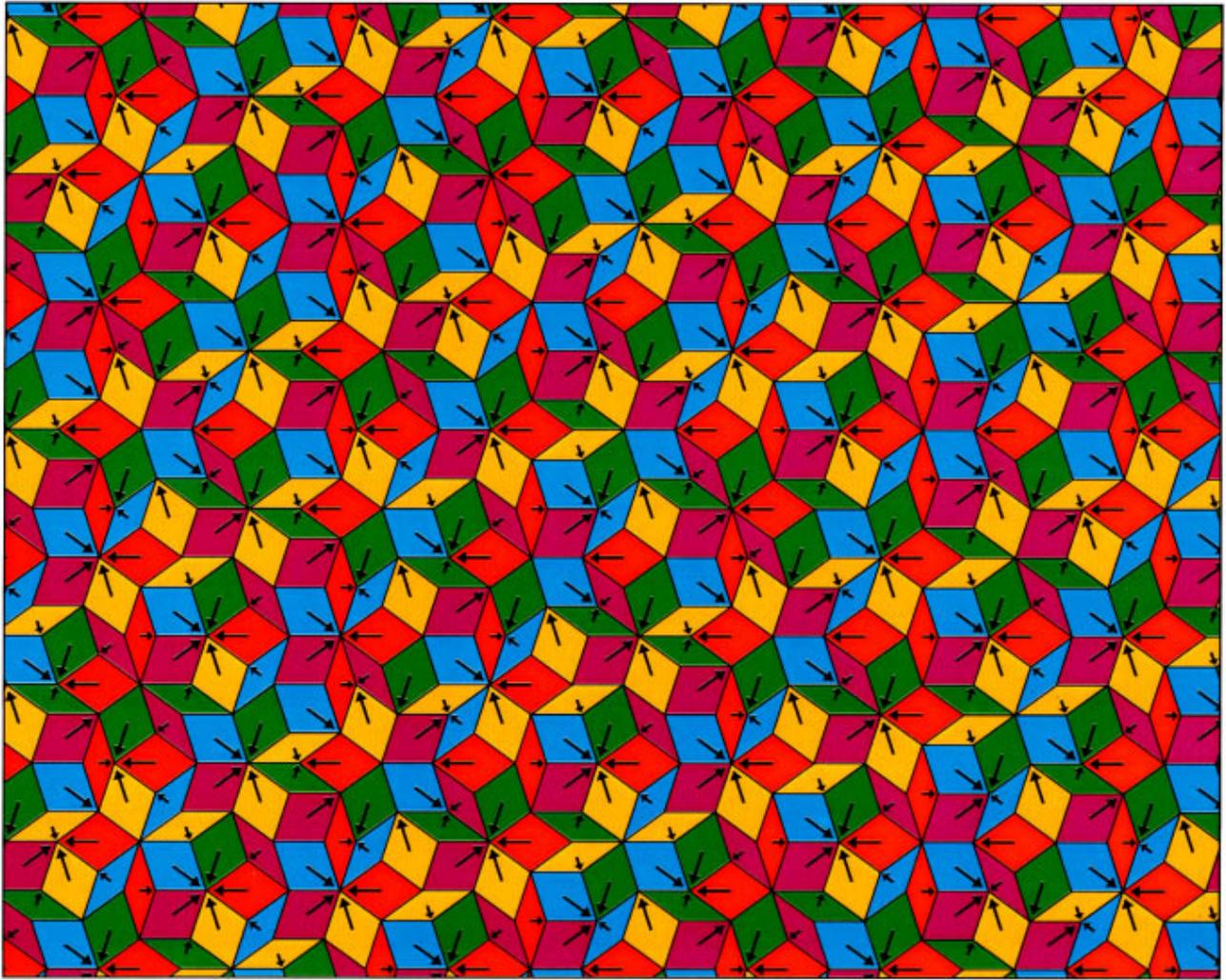


FIG. 4. (Color) A five-color Penrose tiling with color point group  $(10mm, 2mm, 2, 2|Z_1)$ , listed as number 5.a.1 in Table XIII. The colors belong to five different indistinguishability classes containing one color each. In an appropriately chosen gauge the color space group has all phase functions zero everywhere on the lattice. The tiling is created by associating the five colors with the five different orientations of each of the two tiles. Arrows are drawn on the tiles as an example of the way in which colors may represent the different orientations of magnetic moments in a quasicrystalline magnetically ordered crystal.

components of  $\vec{\rho}(\mathbf{r})$ . In general, the lattice  $L$  of the color field is not equal to the lattice  $L_0$  of the color-blind density.

Two color fields are *indistinguishable* if they have identical spatially averaged autocorrelation functions of  $\vec{\rho}(\mathbf{r})$  of any order and for any choice of components,

$$C_{\alpha_1 \dots \alpha_n}^{(n)}(\mathbf{r}_1, \dots, \mathbf{r}_n) = \lim_{V \rightarrow \infty} \frac{1}{V} \int d\mathbf{r} \rho_{\alpha_1}(\mathbf{r}_1 - \mathbf{r}) \dots \rho_{\alpha_n}(\mathbf{r}_n - \mathbf{r}). \quad (6)$$

We prove in the appendix (in a more general context) that an equivalent statement for the indistinguishability of two color fields  $\vec{\rho}(\mathbf{r})$  and  $\vec{\rho}'(\mathbf{r})$  is that their Fourier coefficients are related by

$$\vec{\rho}'(\mathbf{k}) = e^{2\pi i \chi(\mathbf{k})} \vec{\rho}(\mathbf{k}), \quad (7)$$

where a single *gauge function*  $\chi$ , which as in the scalar case of Eq. (3) is linear modulo an integer over the lattice  $L$  of wave vectors, relates *all* the components of the two fields.

## B. Point group and phase functions

Having represented the colored crystal by a color field  $\vec{\rho}(\mathbf{r})$  we are ready for a more formal definition of the point group. We define the *point group*  $G$  of a color field  $\vec{\rho}(\mathbf{r})$  to be the set of all operations  $g$  from  $O(3)$  that leave it indistinguishable to within permutations  $\gamma$  of its components. It is clearly a group because if  $g$  and  $h$  are rotations that satisfy this condition then so are their product and inverses. In general, as we shall later see, there can be many different  $\gamma$ 's associated with each element of  $G$ . We denote physical-space rotations by Latin letters and color permutations by Greek letters. The identity rotation and the identity permutation are denoted by  $e$  and  $\epsilon$ , respectively. We use the same symbol  $\gamma$  to denote an abstract permutation taking one color into another, as in  $\gamma c_i = c_j$ , and to denote the matrix operating on the field  $\vec{\rho}$ , representing this permutation.

According to the definition of indistinguishability, an operation  $g$  is in the point group of  $\vec{\rho}$  if there exists at

least one permutation  $\gamma$  such that all spatially averaged autocorrelation functions constructed out of  $\tilde{\rho}(g\mathbf{r})$  and  $\gamma\tilde{\rho}(\mathbf{r})$  are identical. The equivalent Fourier-space condition for  $g$  to be in the point group  $G$  is that there be a linear gauge function  $\Phi_g^\gamma(\mathbf{k})$  relating  $\tilde{\rho}(g\mathbf{k})$  and  $\gamma\tilde{\rho}(\mathbf{k})$  as in Eq. (7):

$$\tilde{\rho}(g\mathbf{k}) = e^{2\pi i\Phi_g^\gamma(\mathbf{k})} \gamma\tilde{\rho}(\mathbf{k}). \quad (8)$$

As in the scalar case, given by Eq. (4), the gauge functions that are associated in this way with point-group operations are called *phase functions*. In general, there could be many different phase functions associated with a single point-group operation  $g$ , one for each of the corresponding permutations  $\gamma$ .

In the case of periodic crystals one can show [Mermin, 1992, Eq. (2.18)] that any gauge function  $2\pi\chi(\mathbf{k})$ , relating two indistinguishable color fields, is necessarily of the form  $\mathbf{k}\cdot\mathbf{d}$  for some constant vector  $\mathbf{d}$  independent of  $\mathbf{k}$ , so that  $\tilde{\rho}'(\mathbf{r}) = \tilde{\rho}(\mathbf{r} + \mathbf{d})$  and indistinguishability reduces back to identity to within a translation. One can then combine rotations and color permutations with translations to recover the traditional color space groups of periodic crystals, containing operations that satisfy

$$\tilde{\rho}(g\mathbf{r}) = \gamma\tilde{\rho}(\mathbf{r} + \mathbf{d}_g^\gamma), \quad (9)$$

leaving the color field *identical* to what it was. In the quasiperiodic case one must retain the general form of  $\Phi_g^\gamma(\mathbf{k})$ , which is defined only on the lattice and cannot be linearly extended to arbitrary  $\mathbf{k}$ .

### C. The color point group and the color space group

The possible relations between elements of the point group  $G$  and the permutations  $\gamma$ , as we shall see later in Sec. IV, are severely constrained by the point-group condition (8). For now, let us just make the basic observation that if  $(g, \gamma)$  and  $(h, \delta)$  both satisfy condition (8) then it follows from the equality

$$\tilde{\rho}([gh]\mathbf{k}) = \tilde{\rho}(g[h\mathbf{k}]) \quad (10)$$

that so does  $(gh, \gamma\delta)$ . This establishes that the set  $\Gamma$  of all the permutations  $\gamma$  is a group, and that the set of pairs  $(g, \gamma)$  satisfying the point-group condition (8) is also a group. The latter is a subgroup of  $G \times \Gamma$ , which we call the *color point group*  $G_C$ . For each pair  $(g, \gamma)$  in the color point group there is a corresponding phase function  $\Phi_g^\gamma(\mathbf{k})$ . The equality (10) further requires that all the phase functions satisfy the *group compatibility condition*:

$$\forall (g, \gamma), (h, \delta) \in G_C: \quad \Phi_{gh}^{\gamma\delta}(\mathbf{k}) \equiv \Phi_g^\gamma(h\mathbf{k}) + \Phi_h^\delta(\mathbf{k}). \quad (11)$$

In summary, the object that we call the *color space group*, describing the symmetry of a colored crystal, consists of the following three components:

- (1) A lattice of wave vectors  $L$ , characterized by a rank  $D$ , and a point group  $G_L$  under which the lattice is left invariant. Only in the case of periodic crystals is  $L$  reciprocal to a lattice  $T$  of real-space translations

which leave the colored crystal invariant (without requiring any permutation of the colors).

- (2) A *color point group*  $G_C$ , whose elements  $(g, \gamma)$  leave the density of the colored crystal indistinguishable, a criterion which in the case of periodic crystals reduces to identity to within a translation. The *point group*  $G$  of the crystal, containing all the rotations  $g$  that appear in elements of  $G_C$ , is a subgroup of the lattice point group  $G_L$ .
- (3) A *set of phase functions*  $\Phi_g^\gamma(\mathbf{k})$ , one for each pair  $(g, \gamma) \in G_C$ , satisfying the group compatibility condition (11), which only in the periodic case may be given by a corresponding set  $\mathbf{d}_g^\gamma$  of real-space translations in the form  $2\pi\Phi_g^\gamma(\mathbf{k}) = \mathbf{k}\cdot\mathbf{d}_g^\gamma$ .

We continue to call this a color space group even though its spatial part is no longer a subgroup of the Euclidean group  $E(3)$ . Nevertheless, the color space group may be given an algebraic structure of a group of ordered triplets  $(g, \gamma, \Phi_g^\gamma)$ , in a manner similar to that shown originally by Rabson, Ho, and Mermin (1988) and recently again by Dräger and Mermin (1996), in the context of ordinary space groups for uncolored crystals.

## III. THE SYMMETRY CLASSIFICATION SCHEME

There are infinitely many colored crystal structures, each of which has a color space group describing its symmetry. The common symmetry properties of the different structures become clear only after they are classified into properly chosen equivalence classes. We are concerned here with the classification of colored crystals into Bravais classes (Sec. III.A), color geometric crystal classes (Sec. III.B), color arithmetic crystal classes (Sec. III.C), and color space-group types (Sec. III.D).

### A. Bravais classes

Colored crystals as well as uncolored crystals are classified into Bravais classes according to their lattices of wave vectors. Intuitively, two lattices are in the same Bravais class if they have the same rank and point group (to within a spatial reorientation) and if one can “interpolate” between them with a sequence of lattices, all with the same point group and rank. Stated more formally, as presented by Dräger and Mermin (1996), two lattices  $L$  and  $L'$  belong to the same *Bravais class* if:

- (1) The two lattices are isomorphic as Abelian groups, i.e., there is a one-to-one mapping, denoted by a prime ( $'$ ), from  $L$  onto  $L'$ ,

$$\begin{aligned} &': L \rightarrow L' \\ &\mathbf{k} \rightarrow \mathbf{k}' \end{aligned} \quad (12)$$

satisfying

$$(\mathbf{k}_1 + \mathbf{k}_2)' = \mathbf{k}'_1 + \mathbf{k}'_2; \quad (13)$$

- (2) the corresponding lattice point groups  $G_L$  and  $G'_L$  are conjugate subgroups of  $O(3)$ ,

$$G'_L = rG_L r^{-1}, \quad (14)$$

for some proper three-dimensional rotation  $r$ ; and  
(3) the isomorphism (12) between the lattices preserves the actions of their point groups, namely,

$$(g\mathbf{k})' = g'\mathbf{k}', \quad (15)$$

where  $g' = rgr^{-1}$ .

Since the classification of lattices for color vector fields is the same as that for scalar density functions we shall not expand on this issue further but rather refer the interested reader to previous discussions (Mermin, 1992; Mermin and Lifshitz, 1992; Lifshitz, 1995; Dräger and Mermin, 1996).

## B. Color geometric crystal classes

When we say that two colored crystals “have the same color point group” we normally mean that they belong to the same equivalence class of color point groups, called a color geometric crystal class. We say that two  $n$ -color point groups  $G_C$  and  $G'_C$  are in the same *color geometric crystal class* if they are conjugate subgroups of  $O(3) \times S_n$ , where  $S_n$  is the full permutation group of  $n$  colors. This simply means that

$$G'_C = (r, \sigma)G_C(r, \sigma)^{-1}, \quad (16)$$

for some three-dimensional rotation  $r$  and some permutation  $\sigma$ . The effect of the rotation  $r$  on the point group  $G$  is to reorient its symmetry axes in space. The effect of the permutation  $\sigma$  is to “rename” the colors, or to remap the components of the color field to actual colors.

## C. Color arithmetic crystal classes

The concept of a color arithmetic crystal class is used to distinguish between colored crystals that have equivalent lattices and equivalent color point groups but differ in the manner in which the lattice and the color point group are combined. Two colored crystals belong to the same *color arithmetic crystal class* if their lattices are in the same Bravais class, their color point groups are in the same color geometric crystal class, and it is possible to choose the lattice isomorphism [Eq. (12)] such that the proper rotation  $r$  used in Eq. (14) to establish the lattice equivalence is the same rotation used in Eq. (16) to establish the color point-group equivalence.

## D. Color space-group types

The finer classification of crystals in a given color arithmetic crystal class into color space-group types is an organization of sets of phase functions into equivalence classes according to two criteria:

(1) Two *indistinguishable* colored crystals  $\vec{\rho}$  and  $\vec{\rho}'$ , related as in Eq. (7) by a gauge function  $\chi$ , should clearly belong to the same color space-group type. Such crystals are necessarily in the same color arithmetic crystal class but the sets of phase functions  $\Phi$  and  $\Phi'$  used to describe their space groups may, in general, be different.

It follows directly from Eq. (7) and from the point-group condition (8) that two such sets of phase functions are related by

$$\Phi'_{g'}(\mathbf{k}) \equiv \Phi_g(\mathbf{k}) + \chi(g\mathbf{k} - \mathbf{k}), \quad (17)$$

for every  $(g, \gamma)$  in the color point group and every  $\mathbf{k}$  in the lattice. We call two sets of phase functions that describe indistinguishable color fields *gauge-equivalent* and Eq. (17), converting  $\Phi$  into  $\Phi'$ , a *gauge transformation*. The freedom to choose a gauge  $\chi$  by which to transform the Fourier coefficients  $\vec{\rho}(\mathbf{k})$  of the color field and all the phase functions  $\Phi$ , describing a given colored crystal, is associated in the case of periodic colored crystals with the freedom one has in choosing the real-space origin about which all the point-group operations are applied.

(2) Two *distinguishable* colored crystals  $\vec{\rho}$  and  $\vec{\rho}'$ , whose color space groups are given by lattices  $L$  and  $L'$ , color point groups  $G_C$  and  $G'_C$ , and sets of phase functions  $\Phi$  and  $\Phi'$ , have the same color space-group type if they are in the same color arithmetic crystal class and if, to within a gauge transformation (17), the lattice isomorphism (12) taking every  $\mathbf{k} \in L$  into a  $\mathbf{k}' \in L'$  preserves the values of all the phase functions

$$\Phi'_{g'}(\mathbf{k}') \equiv \Phi_g(\mathbf{k}), \quad (18)$$

where  $g' = rgr^{-1}$  and  $\gamma' = \sigma\gamma\sigma^{-1}$ . Two sets of phase functions that are related in this way are called *scale-equivalent*. This nomenclature reflects the fact that the lattice isomorphism (12) used to relate the two lattices may often be achieved by rescaling the wave vectors of one lattice into those of the other.

## IV. ALGEBRAIC STRUCTURE OF THE COLOR SPACE GROUP

In the preceding sections we used the notion of indistinguishability to redefine the concepts of “color point group” and “color space group.” We also described a scheme by which one can classify these groups into meaningful equivalence classes. To this end it was sufficient to use the definition of the color point group as containing all pairs  $(g, \gamma)$  satisfying the point-group condition (8). For dealing with more practical matters, like the enumeration of all color space-group types with a given point group  $G$ , a better understanding of the algebraic structure of the color space group is required. It is the purpose of this section to provide the reader with the necessary details.

In order to simplify some of the points made in this section we shall introduce an additional assumption that the color field is a *generic* one. By this we mean that the color field  $\vec{\rho}$  never has more symmetry than that required by its color space group. The justification for making such an assumption is the practical statement that when classifying color space groups we are not interested in nongeneric cases—the color fields we use should have nothing more than the symmetry properties common to all color fields with the same color space-group type.

In Sec. IV.A we describe the general structure of the color point group. In Sec. IV.B we analyze in more detail the interplay between rotations and color permutations. In Sec. IV.C we investigate the close relation between the lattice color group—a special subgroup of the group  $\Gamma$  of color permutations which will be introduced shortly—and the lattice  $L$  of the crystal. We finish in Sec. IV.D with a comparison of our theory with the traditional theory of color symmetry, used for periodic crystals. The reader might find it helpful to refer throughout this section to Table I below, which lists the various point groups associated with the color field.

### A. Structure of the color point group $G_C$

Recall that the color point group  $G_C$  is a subgroup of  $G \times \Gamma$  with the property that every element of  $G$  and every element of  $\Gamma$  appears in at least one pair of  $G_C$ . Such a subgroup is easily shown to have the following structure:

(1) The set of point-group operations  $G_\epsilon$  associated with the identity of  $\Gamma$  forms a normal subgroup of  $G$ .

*Proof:* Any element  $h \in G$  is paired in  $G_C$  with at least one  $\delta \in \Gamma$ , so  $(h, \delta)$  and its inverse  $(h^{-1}, \delta^{-1})$  are in  $G_C$ . It then follows that if  $(g, \epsilon)$  is in  $G_C$  then so is  $(hgh^{-1}, \epsilon)$ .

*Note:* It follows from successive applications of the group compatibility condition (11) that the corresponding phase functions are related by

$$\forall g \in G_\epsilon, (h, \delta) \in G_C: \quad \Phi_{hgh^{-1}}^\epsilon(h\mathbf{k}) \equiv \Phi_g^\epsilon(\mathbf{k}) + \Phi_h^\delta(g\mathbf{k} - \mathbf{k}). \quad (19)$$

(2) The set of color permutations  $\Gamma_\epsilon$  associated with the identity of  $G$  forms a normal subgroup of  $\Gamma$ . This subgroup of color permutations plays a central role in the enumeration process and is called the *lattice color group* for reasons that will become clear in Sec. IV.C.

*Proof:* The same as the proof of (1) with the roles of  $G$  and  $\Gamma$  interchanged.

*Note:* In this case the corresponding phase functions are related by

$$\forall \gamma \in \Gamma_\epsilon, (h, \delta) \in G_C: \quad \Phi_e^{\delta\gamma\delta^{-1}}(h\mathbf{k}) \equiv \Phi_e^\gamma(\mathbf{k}). \quad (20)$$

(3) The pairs appearing in  $G_C$  associate all the elements of each coset of  $G_\epsilon$  with all the elements of a single corresponding coset of  $\Gamma_\epsilon$ . This correspondence between cosets is an isomorphism between the two quotient groups  $G/G_\epsilon$  and  $\Gamma/\Gamma_\epsilon$ .

*Proof:* One easily verifies for any  $g$  in  $G$  that the elements of  $\Gamma$  paired in  $G_C$  with  $g$  constitute a single coset of  $\Gamma_\epsilon$ . Every coset of  $\Gamma_\epsilon$  is paired with some  $g$  since every element of  $\Gamma$  is paired with some  $g$ . This establishes a map of  $G$  onto the quotient group  $\Gamma/\Gamma_\epsilon$  which is easily seen to be a homomorphism. The kernel of this homomorphism is clearly  $G_\epsilon$ , which establishes the isomorphism of  $G/G_\epsilon$  and  $\Gamma/\Gamma_\epsilon$ .

The group compatibility condition (11) further implies that

(4) The lattice color group  $\Gamma_\epsilon$  is Abelian.

*Proof:* This is established by noting that the phase functions, associated with the elements of  $\{e\} \times \Gamma_\epsilon$ , satisfy

$$\forall \gamma, \delta \in \Gamma_\epsilon: \quad \Phi_e^{\gamma\delta}(\mathbf{k}) \equiv \Phi_e^\gamma(\mathbf{k}) + \Phi_e^\delta(\mathbf{k}), \quad (21)$$

requiring through the point-group condition (8) that  $\gamma\delta\tilde{\rho}(\mathbf{k}) = \delta\gamma\tilde{\rho}(\mathbf{k})$  for every  $\mathbf{k}$ , and therefore that  $\gamma\delta = \delta\gamma$ .

*Note:* It follows directly from Eq. (21) that the complex numbers  $e^{2\pi i\Phi_e^\gamma(\mathbf{k})}$ , for a given  $\mathbf{k}$ , form a one-dimensional representation of  $\Gamma_\epsilon$ .

### B. Relation between rotations and color permutations

#### 1. Point groups associated with the color field

One may characterize the effect of rotations on the color field in a number of ways, each leading to a definition of a different kind of point group. The point group  $G$  of the color field  $\tilde{\rho}(\mathbf{r})$ , for example, is defined as the group of all rotations that leave the color field indistinguishable within a permutation of its components. The normal subgroup  $G_\epsilon$  of  $G$ , introduced above, contains all rotations that leave the color field indistinguishable without requiring any permutation of the components.

By considering in more detail the effect of rotations on the *individual components* of the color field one can define two additional types of point groups which are of practical importance. The first is the point group  $H$  of one of the components of the color field, say, the  $i$ th one. This is the subgroup of  $G$  containing all rotations that leave the scalar function  $\rho_i(\mathbf{r})$  indistinguishable as defined by Eq. (4). The second is the point group  $H_0$  containing all rotations that leave indistinguishable *all* the components of the color field. Clearly,  $H_0$  is a subgroup of  $H$ , and it contains  $G_\epsilon$  as a subgroup. We emphasize that, in general, there may be rotations in  $H_0$  that are not in  $G_\epsilon$ —they leave indistinguishable each individual component of the field but still require a non-trivial permutation of the colors to leave the whole field indistinguishable.

For completeness, one may also consider the point group  $G_0$  of the color-blind density  $\rho_0(\mathbf{r})$ , defined earlier as the sum of the  $n$  components of the color field. But clearly (see Sec. IV.C.3) any rotation in the point group  $G$  of the color field is also in the point group  $G_0$  of the color-blind density. Furthermore, if the color field is generic then there is no reason for  $G_0$  to contain any additional rotations that are not already in  $G$ . Thus we may always assume that  $G_0 = G$ .

Recall that we require that for every two colors, or two components of  $\tilde{\rho}$ , there is at least one permutation in  $\Gamma$  that takes one into the other. The permutation group  $\Gamma$  is said to be *transitive* on the set of colors. This requirement implies, through the point-group condition (8), that every two components of  $\tilde{\rho}(\mathbf{r})$  are indistinguish-

TABLE I. The different point groups associated with a color field. Each group is a subgroup of all the groups listed above it ( $G_\epsilon \subseteq H_0 \subseteq H \subseteq G \subseteq G_0$ ). If the color field is generic then  $G = G_0$ .

Group	Symbol	Effect of the group on the color field
Point group of the color-blind density	$G_0$	Leaves the color-blind density $\rho_0(\mathbf{r}) = \sum_i \rho_i(\mathbf{r})$ indistinguishable.
Point group of the color field	$G$	Leaves the color field $\vec{\rho}(\mathbf{r})$ indistinguishable to within a permutation of its components.
Point group of a single-color density	$H$	Leaves indistinguishable all components $\rho_i(\mathbf{r})$ in a single indistinguishability class.
Largest normal subgroup of $G$ contained in $H$	$H_0$	Leaves all the individual components of the color field indistinguishable.
Kernel of the homomorphism from $G$ to $\Gamma/\Gamma_\epsilon$	$G_\epsilon$	Leaves the color field $\vec{\rho}(\mathbf{r})$ indistinguishable without any permutation of its components.

able as scalar fields to within a spatial rotation. From this it follows that the point groups  $H$  of the different components of the color field are all equivalent—they are all conjugate subgroups of  $G$ . Consequently  $H_0$ , which is the largest subgroup of  $G$  contained in all the subgroups  $H$  for the different choices of colors, may be equivalently defined as the largest *normal* subgroup of  $G$  contained in a particular  $H$ .

The various kinds of point groups associated with the color field are summarized in Table I. The classification of subgroups  $H$  and  $H_0$  for a given point group  $G$  appears also in the traditional theory of color point groups (Senechal, 1975). Such subgroups have been listed by Harker (1976) for all 32 point groups compatible with periodic crystals and for the two icosahedral point groups and are listed below in Table IX for the two-dimensional decagonal and pentagonal point groups. Subgroups  $H$  of index 2 have also been listed for the pentagonal, octagonal, and decagonal point groups by Boyle (1969) and are listed below in Table III for all three-dimensional axial point groups.

## 2. Indistinguishability classes of colors

As a special case of the observation made above, components of the color field that are related by permutations in the lattice color group  $\Gamma_\epsilon$  are required to be indistinguishable as scalar fields even without a rotation because

$$\forall \gamma \in \Gamma_\epsilon: \quad \vec{\rho}(\mathbf{k}) = e^{2\pi i \Phi_\epsilon^\gamma(\mathbf{k})} \gamma \vec{\rho}(\mathbf{k}). \quad (22)$$

It proves useful to arrange the colors into *indistinguishability classes* according to the lattice color group  $\Gamma_\epsilon$ . Two colors  $c_i$  and  $c_j$  are in the same class<sup>4</sup> (denoted by

<sup>4</sup>It might be more accurate to call these “ $\Gamma_\epsilon$  classes” rather than “indistinguishability classes” because there may exist particular color fields in which two components happen to be indistinguishable as scalar fields even though they are *not* related by a permutation in  $\Gamma_\epsilon$ . Nevertheless, recall that we are assuming that when classifying color space groups we are always dealing with generic color fields in which two components are not indistinguishable unless they are required to be so by the color space group.

$c_i \cong c_j$ ) if they are related by a permutation in  $\Gamma_\epsilon$ . We denote the classes by  $C_1 \dots C_q$  where  $q$  is the number of classes. The basic property of these indistinguishability classes is that

*Claim:* Each indistinguishability class contains the same number of colors.

*Proof:* If  $c_i \cong c_j$ , meaning that  $c_i = \gamma c_j$  for some permutation  $\gamma \in \Gamma_\epsilon$ , then

$$\forall \delta \in \Gamma: \quad \delta c_i = \delta \gamma c_j = [\delta \gamma \delta^{-1}] \delta c_j. \quad (23)$$

Because  $\Gamma_\epsilon$  is a normal subgroup of  $\Gamma$  it contains  $\delta \gamma \delta^{-1}$  which implies that  $\delta c_i \cong \delta c_j$ . The permutation  $\delta$  takes all the colors in the class containing  $c_i$  into colors in the class containing  $\delta c_i$ . Similarly,  $\delta^{-1}$  takes all the colors in the class containing  $\delta c_i$  into colors in the class containing  $c_i$ . This establishes that the two classes contain the same number of colors. Because  $\Gamma$  is transitive on the set of colors, the argument above holds for any pair of classes implying that all classes contain the same number  $p$  of colors, so that the total number of colors  $n = pq$ .

One can thus label a given color either as the  $i$ th color  $c_i$  with the index  $i$  ranging from 1 to  $n$ , or as the  $k$ th color in the  $j$ th indistinguishability class  $C_j^k$  with  $j = 1 \dots q$ , and  $k = 1 \dots p$ . From the above proof it follows that any color permutation  $\delta \in \Gamma$  may be viewed as a two-step process, first acting on whole indistinguishability classes, permuting the lower indices of the  $C_j^k$ , and then permuting colors within their indistinguishability classes.

We say that a color point group (or a color space group) is *simple* if for every  $\delta \in \Gamma$  the permutation of colors required within the indistinguishability classes is identical in all classes and can therefore be expressed as a permutation of the upper indices of the  $C_j^k$ . If there is only a single indistinguishability class ( $q = 1$ ) or if all classes contain just a single color ( $p = 1$ ), then the color point group is necessarily simple, otherwise it may be nonsimple. We shall defer to a later publication a detailed analysis of the conditions for crystals in a given Bravais class to be able to accommodate nonsimple color groups. We give an example of a nonsimple color space group in Sec. IV.C.6.

### 3. Point-group rotations and permutations of indistinguishability classes

It follows directly from the definition of the indistinguishability classes that two color permutations in the same coset of  $\Gamma_e$  necessarily induce the same permutation of the indistinguishability classes. Note that the converse is not true because, even though all the permutations in  $\Gamma_e$  permute colors only within their indistinguishability class, not every permutation that does so is necessarily in  $\Gamma_e$ . Any point-group rotation  $h$  is paired in the color point group with all the permutations in a single coset  $\delta\Gamma_e$ , all inducing the same permutation of the indistinguishability classes. In fact, the effect of applying  $h$  on the color field without following up with one of the color permutation in  $\delta\Gamma_e$  is to permute the indistinguishability classes according to the permutation induced by the elements of the coset  $\delta^{-1}\Gamma_e$ . One can therefore sensibly associate indistinguishability-class permutations with point-group rotations.

The mapping between the point group  $G$  and the set of indistinguishability-class permutations, induced by the elements of  $\Gamma$ , is clearly a homomorphism because the mapping between  $G$  and the cosets of  $\Gamma_e$  is a homomorphism. The kernel of this homomorphism is the subgroup  $H_0$ , containing all rotations that leave all the components of the color field indistinguishable. The color permutations that are then required in order to leave the whole color field indistinguishable permute colors only within their indistinguishability classes and therefore induce the identity permutation of the indistinguishability classes. Rotations in  $H$  leave indistinguishable the density of a given color and are therefore paired in the color point group with permutations that permute that particular color only within its indistinguishability class. The rotations in  $H$  are therefore associated with cosets of  $\Gamma_e$  that induce indistinguishability-class permutations which leave invariant a *single* indistinguishability class but may otherwise nontrivially permute all the other classes.

Following similar ideas of Senechal's (1975) one can establish a clear connection between the cosets of  $H$  and the indistinguishability classes of the colors. Choosing an indistinguishability class, say  $C_1$ , defines  $H$  as the point group of all the components of the color field belonging to that class. One can verify that two rotations are in the same left coset of  $H$  if and only if the permutations of the indistinguishability classes associated with these rotations both take  $C_1$  into the same class. There are thus as many cosets as there are indistinguishability classes—each coset  $g_iH$  corresponds to a single class  $C_i$  and the number  $q$  of indistinguishability classes is therefore equal to the index of  $H$  in  $G$ . Multiplying each coset of  $H$  by any rotation  $g$  in  $G$  induces a permutation of the cosets and therefore a corresponding permutation of the indistinguishability classes. Thus  $H$  determines the permutation group of the indistinguishability classes, which, as established above, is isomorphic to  $G/H_0$ . In the special case when  $H$  is itself a normal subgroup of  $G$  and

therefore equal to  $H_0$ , the order of the quotient group  $G/H_0$  is equal to the number of indistinguishability classes.

In summary, the  $n$  colors are arranged into  $q$  indistinguishability classes each containing  $p$  colors. Any color permutation may be viewed as first permuting whole indistinguishability classes of colors and then permuting the colors within their classes. The subgroup  $H$  of  $G$ , describing the point-group symmetry of one component of the color field, uniquely determines the indistinguishability-class permutation associated with each rotation  $g \in G$ . This is due to the correspondence between the  $q$  indistinguishability classes and the  $q$  left cosets of  $H$  in  $G$ . In the next section we shall establish how one determines the additional permutation for a given  $g$ , which is required within the indistinguishability classes to leave the color field indistinguishable.

### C. Relation between the lattice $L$ and the lattice color group $\Gamma_e$

Let us focus now on the normal Abelian subgroup  $\Gamma_e$ . It contains all the color permutations  $\gamma$  that leave the color field indistinguishable without requiring any rotation in physical space. In the special case of periodic crystals, these are color permutations that when combined with a translation leave the colored crystal invariant. The phase functions  $\Phi_e^{\gamma}(\mathbf{k})$  therefore contain the information that generalizes to the quasiperiodic case the concept of a “colored lattice,” also called a “color translation group,” or “color lattice group.”<sup>5</sup> We choose to call  $\Gamma_e$  the *lattice color group* because, as we shall show in this section, it is a group of color permutations which even in the quasiperiodic case is closely related to the lattice  $L$  of wave vectors.

Recall that the lattice itself is an Abelian group, with vector addition as the group composition law. We shall show that there exists a sublattice  $L_0$  of  $L$  for which the modular lattice (or quotient group)  $L/L_0$ , in which vector addition is performed modulo vectors in  $L_0$ , is isomorphic to  $\Gamma_e$ . We shall shortly define  $L_0$ , then prove the isomorphism between  $L/L_0$  and  $\Gamma_e$ , and then show that  $L_0$  is none other than the lattice of the color-blind density, first introduced in Sec. II.A. We shall then proceed to show that the isomorphism  $L/L_0 \cong \Gamma_e$  is invariant under the full color point group, which imposes an additional constraint on the lattice color group  $\Gamma_e$  and also determines the nature of all color permutations that are paired in the color point group with a given rotation. But first, let us review the properties of the phase functions associated with the elements of  $\{e\} \times \Gamma_e$ .

<sup>5</sup>For the precise definition and use of these concepts in the traditional theory of color symmetry for periodic crystals see, for example, Harker (1978a; 1978b) or Opechowski (1986, Sec. 13.4.1).

1. Properties of the phases  $\Phi_e^\gamma(\mathbf{k})$ 

(1) *Gauge invariance.* All phase functions of the form  $\Phi_e^\gamma$  are independent of the choice of gauge—they are left invariant under any gauge transformation (17).

(2) *Linearity on the lattice  $L$ .* This is a property of all phase functions, in particular,

$$\forall \gamma \in \Gamma_e: \quad \Phi_e^\gamma(\mathbf{k}_1 + \mathbf{k}_2) \equiv \Phi_e^\gamma(\mathbf{k}_1) + \Phi_e^\gamma(\mathbf{k}_2), \quad \mathbf{k}_1, \mathbf{k}_2 \in L. \quad (24)$$

(3) *Linearity on the group  $\Gamma_e$ .* The group compatibility condition (11) for the phases  $\Phi_e^\gamma(\mathbf{k})$  states that  $\forall \mathbf{k} \in L$ :

$$\Phi_e^{\gamma_1 \gamma_2}(\mathbf{k}) \equiv \Phi_e^{\gamma_1}(\mathbf{k}) + \Phi_e^{\gamma_2}(\mathbf{k}), \quad \gamma_1, \gamma_2 \in \Gamma_e. \quad (25)$$

Thus, for any fixed  $\mathbf{k}$ , the phases  $\Phi_e^\gamma(\mathbf{k})$  are a linear function on  $\Gamma_e$  in the sense that the group composition law of  $\Gamma_e$  can be expressed as addition (because  $\Gamma_e$  is Abelian).

(4) *Possible values.* Because  $\Gamma_e$  is a finite group it has an *exponent*  $m$ , which is the smallest integer satisfying  $\gamma^m = \epsilon$  for every  $\gamma$  in  $\Gamma_e$ . It then follows from the group compatibility condition (25) that

$$\forall \mathbf{k} \in L, \gamma \in \Gamma_e: \quad \Phi_e^\gamma(\mathbf{k}) \equiv \frac{j}{m}, \quad j = 0, 1, \dots, m-1. \quad (26)$$

(5) *Invariance under the full color point group  $G_C$ .* The lattice  $L$  is invariant under the point group  $G$ ; the group  $\Gamma_e$  is invariant under the full permutation group  $\Gamma$ ; from successive applications of the group compatibility condition (11) we find that

$$\forall \mathbf{k} \in L, \gamma \in \Gamma_e: \quad \Phi_e^{\delta \gamma \delta^{-1}}(h\mathbf{k}) \equiv \Phi_e^\gamma(\mathbf{k}), \quad (h, \delta) \in G_C, \quad (27)$$

which may be interpreted as saying that the phases  $\Phi_e^\gamma(\mathbf{k})$  are invariant under the full color point group  $G_C$ .

Properties (1) through (4) imply that the phase functions  $\Phi_e^\gamma(\mathbf{k})$  provide a gauge-invariant bilinear mapping from  $L \times \Gamma_e$  into  $Z_m$ —the cyclic group of order  $m$ . Most of the structural relation between the lattice  $L$  and the lattice color group  $\Gamma_e$ , described below, is a general consequence of having such a bilinear mapping (for more details, see for example Lang, 1971, Sec. I§11). Property (5) imposes the symmetry of the full color point group on the bilinear mapping which in turn adds a further requirement on the structural relation between  $L$  and  $\Gamma_e$ .

2. Proof of isomorphism between  $L/L_0$  and  $\Gamma_e$ 

The group  $Z_m$ , which is represented above as the addition modulo 1 of fractions with denominator  $m$ , may also be represented in exponential form as the product of the  $m$ th roots of unity  $e^{2\pi i \Phi_e^\gamma(\mathbf{k})}$ . In the latter form, property (3) states that the phase functions define a mapping  $\phi$  from the lattice  $L$  to the set  $IR(\Gamma_e)$  of irre-

ducible representations of  $\Gamma_e$ . That is, every wave vector  $\mathbf{k}$  is associated with one of the irreducible representations of  $\Gamma_e$ . One can easily convince oneself that the set of irreducible representations of a finite Abelian group, all of which are one dimensional, is itself a group. Consequently, property (2) establishes in addition that  $\phi$  is actually a group homomorphism from  $L$  to  $IR(\Gamma_e)$ . That is, the representation associated with the wave vector  $\mathbf{k}_1 + \mathbf{k}_2$  is the product of the two representations associated with  $\mathbf{k}_1$  and  $\mathbf{k}_2$ .

Let  $L_0$  be the kernel of this homomorphism—the sublattice containing all wave vectors  $\mathbf{k}$  that are mapped to the identity representation of  $\Gamma_e$  or, equivalently, for which all phases  $\Phi_e^\gamma(\mathbf{k}) \equiv 0$ . The mapping  $\phi$  is then a homomorphism

$$\phi: L/L_0 \rightarrow IR(\Gamma_e) \quad (28)$$

which is injective—all wave vectors in a single coset of  $L_0$  are mapped to the same representation of  $\Gamma_e$ , and any two wave vectors that belong to different cosets of  $L_0$  are mapped to distinct representations of  $\Gamma_e$ . This implies that

$$|L/L_0| \leq |IR(\Gamma_e)| = |\Gamma_e|, \quad (29)$$

where  $|\dots|$  denotes the order of a group, and the equality on the right is a property of any finite Abelian group.

Exchanging the roles of  $L$  and  $\Gamma_e$ , one similarly finds, using properties (2) and (3), that the phase functions define an injective homomorphism

$$\psi: \Gamma_e \rightarrow IR(L/L_0) \quad (30)$$

and so

$$|\Gamma_e| \leq |IR(L/L_0)| = |L/L_0|. \quad (31)$$

From Eqs. (29) and (31) it follows that the orders of  $\Gamma_e$  and  $L/L_0$  are equal and therefore that  $\phi$  and  $\psi$  are actually isomorphisms.

We complete the proof that  $L/L_0$  and  $\Gamma_e$  are isomorphic by noting that any finite Abelian group is isomorphic to its group of irreducible representations.<sup>6</sup> Thus the isomorphism of  $L/L_0$  and  $\Gamma_e$  is established via their corresponding groups of irreducible representations.

3.  $L_0$  is the lattice of the color-blind density

Recall that the color-blind density  $\rho_0$  is defined as the sum of all the components of  $\vec{\rho}$ . By summing the components on the two sides of the point-group condition (8),

$$\forall (g, \gamma) \in G_C: \quad \rho_0(g\mathbf{k}) = e^{2\pi i \Phi_g^\gamma(\mathbf{k})} \rho_0(\mathbf{k}), \quad (32)$$

<sup>6</sup>Since any finite Abelian group may be expressed as a product of cyclic groups, and since by simple inspection any cyclic group is isomorphic to its group of irreducible representations, all that one is left to show is that if  $A$  and  $B$  are two finite Abelian groups then  $IR(A \times B)$  is isomorphic to  $IR(A) \times IR(B)$ . For details see the discussion on dual groups by Lang (1971, Sec. I§11).

one finds, as expected, that any rotation in  $G$  is also in the point group of the color-blind density. *A priori*, we expect any wave vector  $\mathbf{k}$  in  $L$  to be in the lattice of the color-blind density unless the sum of the components of  $\tilde{\rho}(\mathbf{k})$  happens to vanish systematically at a subset of the  $\mathbf{k}$ 's so as to reduce  $L$  to one of its sublattices. To determine for which  $\mathbf{k}$ 's  $\rho_0(\mathbf{k})$  vanishes one needs to examine the color point group symmetries of the form  $(e, \gamma)$ . For, as can be seen from Eq. (32), if  $g=e$  then

$$\forall \mathbf{k} \in L: \rho_0(\mathbf{k}) = e^{2\pi i \Phi_e^\gamma(\mathbf{k})} \rho_0(\mathbf{k}), \quad (33)$$

which directly implies that  $\rho_0(\mathbf{k})$  must vanish unless  $\Phi_e^\gamma(\mathbf{k}) \equiv 0$  for all  $\gamma$  in  $\Gamma_e$ . This is just the set of wave vectors that are mapped to the identity representation of  $\Gamma_e$  and form the sublattice  $L_0$ . Thus  $L_0$ , defined earlier as the kernel of the mapping  $\phi$  from  $L$  to  $IR(\Gamma_e)$ , is in fact the lattice of the color-blind density.<sup>7</sup>

#### 4. Canonical choice of generators for the lattice color group $\Gamma_e$

We have established that the following groups are all isomorphic:

- (1) The lattice color group  $\Gamma_e$ ;
- (2) the modular lattice  $L/L_0$ ;
- (3) the set of all phase functions  $\phi_e^\gamma(\mathbf{k})$ , one for every  $\gamma \in \Gamma_e$ , acting as the group of irreducible representations of the modular lattice  $L/L_0$ ; and
- (4) the sets of phase values  $\{\phi_e^{\gamma_1}(\mathbf{k}), \phi_e^{\gamma_2}(\mathbf{k}), \dots\}$ , one set for every  $\mathbf{k} \in L/L_0$ , acting as the group of irreducible representations of the lattice color group  $\Gamma_e$ .

Let  $\mathbf{b}_1 \dots \mathbf{b}_l$  be a chosen set of independent generators for the modular lattice, and let  $m_1 \dots m_l$  be their corresponding orders (i.e.,  $m_i$  is the smallest integer such that  $m_i \mathbf{b}_i \in L_0$ ). We would like to introduce a *canonical choice* of generators  $\gamma_1 \dots \gamma_l$  for the lattice color group.

Because the values of all phase functions on the vectors of the sublattice  $L_0$  are zero, we have  $\forall \gamma \in \Gamma_e: m_i \Phi_e^\gamma(\mathbf{b}_i) \equiv 0$ , or

$$\forall \gamma \in \Gamma_e: \Phi_e^\gamma(\mathbf{b}_i) \equiv 0, \frac{1}{m_i}, \frac{2}{m_i} \dots \frac{m_i-1}{m_i}. \quad (34)$$

We choose the generators  $\gamma_1 \dots \gamma_l$ , with corresponding orders  $m_1 \dots m_l$  such that their phase functions correspond to the irreducible representations of the modular lattice that are given by

$$\Phi_e^{\gamma_i}(\mathbf{b}_j) \equiv \frac{1}{m_j} \delta_{ij} \quad i, j = 1 \dots l, \quad (35)$$

<sup>7</sup>Operations of the form  $(g, \gamma)$  for  $g \neq e$  may require  $\rho_0(\mathbf{k})$  to vanish at additional wave vectors  $\mathbf{k}$  but only if they lie in the invariant subspace of  $g$ . These additional wave vectors will, nevertheless, remain in the lattice due to its closure under vector addition. This has been proven by Lifshitz (1996b) in the context of spin-density fields. The proof in the case of color fields should be similar.

where  $\delta_{ij}$  is the Kronecker delta. One may easily verify that these  $l$  distinct phase functions, which must exist due to the isomorphism of the first three groups above, indeed generate the complete set of phase functions. The color permutations  $\gamma_1 \dots \gamma_l$  are therefore a valid set of generators for the lattice color group  $\Gamma_e$ .

We have thus established that, for a given lattice  $L$  and a given point group  $G$ , the determination of the *abstract structure* of all the compatible lattice color groups  $\Gamma_e$  along with the values of their associated phase functions  $\Phi_e^\gamma(\mathbf{k})$  is equivalent to the characterization of all distinct sublattices  $L_0$  of  $L$  that are invariant under  $G$  and can play the role of the lattice of the color-blind density. We emphasize that the sublattice  $L_0$  determines the group  $\Gamma_e$  only to within an isomorphism. There could still be different lattice color groups  $\Gamma_e$  that are isomorphic. We shall see next how the requirement that the isomorphism between  $L/L_0$  and  $\Gamma_e$  be invariant under the full color point group (a) may further restrict the possible lattice color groups that are compatible with  $L$  and  $G$  and (b) determines the nature of the color permutation, paired in the color point group with a given rotation.

#### 5. Invariance of the isomorphism of $L/L_0$ and $\Gamma_e$ under the color point group

We have established in Sec. IV.B that identifying the subgroup  $H$  of  $G$  uniquely determines the indistinguishability-class permutation, induced by permutations  $\delta$  which are paired with a rotation  $h \in G$ , according to the effect of  $h$  on the left cosets of  $H$  in  $G$ . We have shown here that identifying the invariant sublattice  $L_0$  of  $L$  determines the abstract structure of  $\Gamma_e$  and its associated phase functions. We shall now establish that the invariance of the isomorphism  $L/L_0 \cong \Gamma_e$  under the full color point group  $G_C$  determines the way in which permutations  $\delta$  are further required to permute colors within their indistinguishability classes, uniquely identifying the coset of  $\Gamma_e$  paired in  $G_C$  with  $h$ .

Let  $(h, \delta)$  be any operation in the color point group  $G_C$ . It then follows from the invariance [Eq. (27)] of the phases  $\Phi_e^\gamma(\mathbf{k})$  under  $G_C$  that the one-dimensional representation of  $\Gamma_e$  associated with  $\mathbf{k}$  assigns the same characters to the elements  $\gamma$  as does the representation associated with  $h\mathbf{k}$  to the elements  $\delta\gamma\delta^{-1}$ . Two such representations of  $\Gamma_e$  are said to be conjugate to each other relative to  $\Gamma$ . The permutation  $\delta$  induces an automorphism on the group  $IR(\Gamma_e)$  of irreducible representations of  $\Gamma_e$  through the corresponding automorphism it induces on the group  $\Gamma_e$  itself. So, if  $\mathbf{k} \in L/L_0$  is mapped by the isomorphism  $L/L_0 \cong \Gamma_e$  to an element  $\gamma \in \Gamma_e$  through some representation of  $\Gamma_e$  then  $h\mathbf{k}$  is mapped through a conjugate representation to the conjugate element  $\delta\gamma\delta^{-1} \in \Gamma_e$ . This is the sense in which the isomorphism between  $L/L_0$  and  $\Gamma_e$  is invariant under the color point group.

A necessary condition for satisfying the invariance of the isomorphism  $L/L_0 \cong \Gamma_e$  under  $G_C$  is that the arrangement of vectors in  $L/L_0$  into stars or orbits of the

point group  $G$  corresponds to a similar arrangement of the elements of  $\Gamma_e$  into orbits of the full permutation group  $\Gamma$ . Because  $\Gamma_e$  is a normal subgroup of  $\Gamma$  all the color permutations in  $\Gamma$  are taken from the group of automorphisms of  $\Gamma_e$ —the set of all color permutations that leave  $\Gamma_e$  invariant. The invariance of the isomorphism  $L/L_0 \cong \Gamma_e$  under  $G_C$  determines which of these color permutations are paired in the color point group with a given rotation  $h$ . These are the permutations that produce the automorphism of  $\Gamma_e$  required by the effect of  $h$  on the modular lattice  $L/L_0$ .

6. Consequences and examples

Let us illustrate the ideas of this section with the help of two examples, both involving two-dimensional four-colored periodic crystals, the first on a square lattice and the second on a triangular lattice. The lattice  $L$  is generated by two wave vectors of equal length,  $\mathbf{b}_1$  and  $\mathbf{b}_2$ , separated in the first case by 90 degrees and in the second case by 120 degrees. Let us restrict ourselves to the simplest point group generated by a single rotation  $r$ , which in the first case is a fourfold rotation and in the second case a threefold rotation.

Let  $L_0$  be the sublattice generated by  $2\mathbf{b}_1$  and  $2\mathbf{b}_2$  (containing all points indexed by a pair of even integers). The modular lattice (or quotient group)  $L/L_0$  is isomorphic to  $\mathbb{Z}_2 \times \mathbb{Z}_2$ , containing the four elements: 0,  $\mathbf{b}_1$ ,  $\mathbf{b}_2$ , and  $\mathbf{b}_1 + \mathbf{b}_2$ . Let us denote the corresponding elements of  $\Gamma_e$  by  $\epsilon$ ,  $\gamma_1$ ,  $\gamma_2$ , and  $\gamma_{12} = \gamma_1 \gamma_2$ ; and the irreducible representations of  $\mathbb{Z}_2 \times \mathbb{Z}_2$  by  $\Delta_0$ ,  $\Delta_1$ ,  $\Delta_2$ , and  $\Delta_{12} = \Delta_1 \Delta_2$ . The color point group may be generated by the three elements:  $(e, \gamma_1)$ ,  $(e, \gamma_2)$ , and  $(r, \delta)$ , where  $\delta$  is a representative of the coset of  $\Gamma_e$ , paired with  $r$  in the color point group.

One can verify from the character table

	$\epsilon$	$\gamma_1$	$\gamma_2$	$\gamma_{12}$	
$\Delta_0$	1	1	1	1	
$\Delta_1$	1	-1	1	-1	
$\Delta_2$	1	1	-1	-1	
$\Delta_{12}$	1	-1	-1	1	(36)

that it is always possible, through a renaming of the elements of  $\Gamma_e$ , to assign the representations  $\Delta_1$  and  $\Delta_2$  to the wave vectors  $\mathbf{b}_1$  and  $\mathbf{b}_2$ , respectively. By renaming we mean choosing which two elements to call  $\gamma_1$  and  $\gamma_2$  and use as generators of the group. Any of the other five possible assignments will lead to equivalent color space groups, as defined in Sec. III.D. Furthermore, one can easily show, in both the square and the triangular cases, that there exists a gauge [Eq. (17)] in which the phase function  $\Phi_r^\delta(\mathbf{k})$  is zero everywhere on the lattice  $L$ .

Stated explicitly, the phase functions associated with the generators of the color point group, to within a gauge transformation (17) and a renaming of the elements of  $\Gamma_e$ , are

$$\begin{aligned} \Phi_e^{\gamma_1}(\mathbf{b}_1) &\equiv \frac{1}{2}, & \Phi_e^{\gamma_1}(\mathbf{b}_2) &\equiv 0, \\ \Phi_e^{\gamma_2}(\mathbf{b}_1) &\equiv 0, & \Phi_e^{\gamma_2}(\mathbf{b}_2) &\equiv \frac{1}{2}, \\ \Phi_r^\delta(\mathbf{b}_1) &\equiv 0, & \Phi_r^\delta(\mathbf{b}_2) &\equiv 0. \end{aligned} \tag{37}$$

Thus choosing  $L_0$  not only determines the abstract structure of  $\Gamma_e$  but also determines the assignment of phases to the corresponding phase functions. Up to this point both the square and the triangular crystals behave in the same manner. They differ in the actual lattice color groups  $\Gamma_e$  that are allowed due to the requirement that the isomorphism between the modular lattice  $L/L_0$  and  $\Gamma_e$  be invariant under the respective color point groups. The different lattice color groups, derived below for the two cases, are illustrated in Fig. 5.

The fourfold rotation interchanges  $\mathbf{b}_1$  and  $\mathbf{b}_2$  (modulo vectors in  $L_0$ ) so any permutation  $\delta$ , paired in the color group with  $r$ , must interchange  $\gamma_1$  and  $\gamma_2$ . There are two possible lattice color groups satisfying this requirement:

	$\gamma_1$	$\gamma_2$	$\gamma_{12}$	$\delta$
1.	$(c_1 c_2)(c_3 c_4)$	$(c_1 c_3)(c_2 c_4)$	$(c_1 c_4)(c_2 c_3)$	$(c_2 c_3)$
2.	$(c_1 c_2)$	$(c_3 c_4)$	$(c_1 c_2)(c_3 c_4)$	$(c_1 c_4)(c_2 c_3)$

This gives two different four-color square space groups with point group  $G=4$  and with the chosen sublattice  $L_0$ . Note that in the first case the four colors belong to a single indistinguishability class whereas in the second they belong to two different indistinguishability classes. The second case is an example of a nonsimple color space group, as defined in Sec. IV.B.2.

The threefold rotation, on the other hand, cyclically permutes the three vectors  $\mathbf{b}_1$ ,  $\mathbf{b}_2$ , and  $\mathbf{b}_1 + \mathbf{b}_2$ . A permutation  $\delta$ , paired in the color group with  $r$ , must cyclically permute the three elements  $\gamma_1$ ,  $\gamma_2$ , and  $\gamma_{12}$ . There is only one lattice color group satisfying this requirement:

	$\gamma_1$	$\gamma_2$	$\gamma_{12}$	$\delta$
1.	$(c_1 c_2)(c_3 c_4)$	$(c_1 c_3)(c_2 c_4)$	$(c_1 c_4)(c_2 c_3)$	$(c_2 c_3 c_4)$

The second possibility on the square lattice is not possible on the triangular lattice because the fact that the three vectors  $\mathbf{b}_1$ ,  $\mathbf{b}_2$ , and  $\mathbf{b}_1 + \mathbf{b}_2$  belong to the same orbit of the point group requires the three elements  $\gamma_1$ ,  $\gamma_2$ , and  $\gamma_{12}$  to be conjugate in  $\Gamma$ . Thus there is only a single four-color trigonal space group with point group  $G=3$  with this choice for the sublattice  $L_0$ .

D. Relation to the traditional theory of color symmetry

The standard procedure in the case of periodic color space groups, as presented, for example, by Senechal (1975; 1979), Schwarzenberger (1984), or Opechowski (1986), is to formulate the problem in terms of subgroups of space groups. After fixing the origin in real space, one assigns to each element of a space group  $\mathcal{G}$  (including its translations) a unique permutation  $\gamma$  of the  $n$  colors required to leave the colored crystal invariant. This defines a homomorphism from  $\mathcal{G}$  onto the permu-

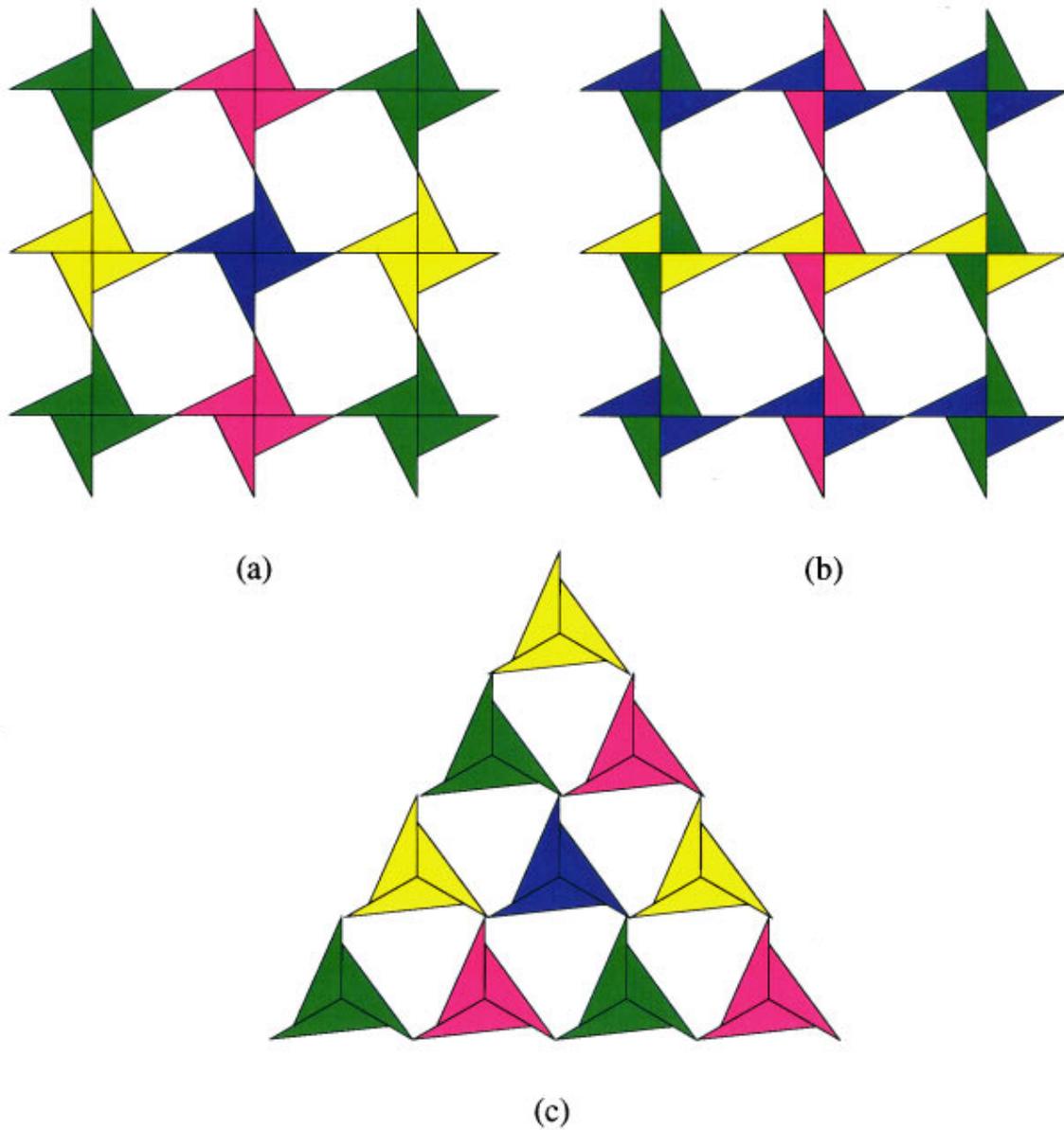


FIG. 5. (Color) Illustration of four-color space groups with lattice color groups isomorphic to  $Z_2 \times Z_2$ . With fourfold symmetry there are two possibilities for lattice color groups, (a) generated by  $\gamma_1 = (c_1 c_2)(c_3 c_4)$  and  $\gamma_2 = (c_1 c_3)(c_2 c_4)$  or (b) generated by  $\gamma_1 = (c_1 c_2)$  and  $\gamma_2 = (c_3 c_4)$ . With threefold symmetry only the first possibility can be realized, as shown in (c).

tation group  $\Gamma$ . The elements of  $\mathcal{G}$  associated with permutations that leave a given color  $c_1$  invariant form a subgroup  $\mathcal{H}$  of index  $n$  in  $\mathcal{G}$ . The elements of  $\mathcal{G}$  associated with permutations that take color  $c_1$  into color  $c_k$  form a left coset of  $\mathcal{H}$ , and there is a correspondence between cosets of  $\mathcal{H}$  and colors. The permutation  $\gamma$  associated with a given element  $g$  of  $\mathcal{G}$  is determined by the permutation of the left cosets of  $\mathcal{H}$  induced by  $g$ . Because  $\Gamma$  is determined uniquely by  $\mathcal{H}$  (up to a relabeling of the colors and a global shift of the origin), the color space group is denoted by the group-subgroup pair  $\mathcal{G}(\mathcal{H})$ .

If  $\mathcal{H}$  and  $\mathcal{G}$  share the same lattice of translations they are called *translation equivalent* and if they have the same point group they are called *class equivalent*. According to a theorem by Hermann (Senechal, 1990, p.

72) every subgroup of a space group that is of finite index is a translation-equivalent subgroup of a class-equivalent subgroup. This allows one to split the enumeration problem into two, considering colored lattices (in terms of sublattices of lattices of translations) and color point groups (in terms of subgroups of point groups) and composing them to construct the color space groups.

Our theory, based on the Fourier-space approach, does not deal with translations, making it equally applicable to periodic and to quasiperiodic crystals. The emphasis is shifted from combinations of rotations and translations that leave the crystal invariant to rotations that leave it indistinguishable. Consequently a given point-group rotation is not associated with a unique permutation of the colors but rather with a whole coset of

permutations with which it may be combined to leave the crystal indistinguishable. Alternatively, each point-group rotation is associated with a unique permutation of whole indistinguishability classes of colors, followed by any one of the permutations of colors within their indistinguishability classes that produces the desired automorphism of the lattice color group  $\Gamma_e$ .

One can readily identify the space groups  $\mathcal{G}$  and  $\mathcal{H}$  in our theory as the space group of the color-blind density  $\rho_0(\mathbf{r})$  and the space group of a single component  $\rho_i(\mathbf{r})$  of the color field, respectively. In the periodic case color permutations associated with pure translations are those which leave the color field indistinguishable without requiring any rotation, constituting the lattice color group  $\Gamma_e$ . The enumeration of color Bravais classes in the periodic case is therefore equivalent to the enumeration of the distinct lattice color groups  $\Gamma_e$ , compatible with lattices in a given ordinary Bravais class.

Translation-equivalent color groups are those for which  $\Gamma_e$  contains only the identity permutation. In these color groups  $L=L_0$ , each indistinguishability class contains just a single color ( $p=1$ ), and the subgroups  $H_0$  and  $G_e$  are equal (because in such a case if you leave all the individual components of the field indistinguishable then you necessarily leave the whole field indistinguishable).

Class-equivalent color groups are those for which  $G=H(=H_0)$ , requiring that there be only a single indistinguishability class of colors ( $q=1$ ). These are also the color groups for which the lattices  $L_i$  of the individual components  $\rho_i$  of the color field are necessarily all equal, containing the same set of wave vectors. In general, these lattices are required to be equal only to within rotations in the point group.

## V. BLACK AND WHITE SPACE GROUPS

Though in many ways quite trivial, black and white space groups still deserve careful consideration since they are probably the most important when it comes to applications. The color field  $\vec{\rho}(\mathbf{r})$  has two components corresponding to a black density and a white density. The permutation group  $\Gamma$  is the simplest one possible, containing the identity  $\epsilon$  and the exchange of black and white, which we denote by  $\gamma$ . Tables of periodic black and white space-group types—also known as “Shubnikov groups” or “magnetic groups”—in two and three dimensions are given by Shubnikov and Belov (1964, Tables 10 and 11), Opechowski (1986, Tables 11.2 and 17.3), and the original papers cited therein. We shall outline some general considerations regarding black and white groups, after which we shall enumerate all two- and three-dimensional black and white space-group types on standard axial lattices and the black and white space-group types in the icosahedral system.

### A. General considerations

There are two kinds of black and white space groups depending on the lattice color group  $\Gamma_e$ . In the first,  $\Gamma_e$

contains only the identity permutation, and the two components of the color field are distinguishable. In the second,  $\Gamma_e$  contains  $\gamma$  as well, and the two colors belong to a single indistinguishability class. In both cases the subgroups  $H$ ,  $H_0$ , and  $G_e$  of the point group  $G$  are all equal. One is usually interested in enumerating all the black and white space-group types with a lattice  $L$  from a given Bravais class and a point group  $G$  compatible with that Bravais class. The enumeration proceeds differently depending on the lattice color group  $\Gamma_e$  as outlined below.

1. The colors are distinguishable ( $\Gamma=\{\epsilon, \gamma\}$ ;  $\Gamma_e=\{\epsilon\}$ ;  
 $\Gamma/\Gamma_e \simeq \mathbb{Z}_2$ )

#### a. Color geometric crystal classes

Because  $G/G_e$  is isomorphic to  $\Gamma/\Gamma_e$ , which is isomorphic to  $\mathbb{Z}_2$ , one needs to consider all subgroups  $G_e$  of index 2 of the point group of interest  $G$ . Elements in  $G_e$  are paired in the color point group only with the identity permutation  $\epsilon$ , the rest of the elements being paired only with the exchange of black and white  $\gamma$ . Consequently there is just one element in the black and white point group  $G_C$  associated with each element of  $G$ . One can specify the black and white point group  $G_C$  in any of the following ways: (1) by listing the group-subgroup pair  $G(G_e)$ ; (2) by giving a set of elements that generate  $G_C$ ; or (3) by using the international (Hermann-Mauguin) symbol for the point group  $G$  (e.g., International Union of Crystallography, 1995, Sec. 2.4) and denoting by a prime each element that is paired with  $\gamma$  in  $G_C$ .

A simple way of finding all the subgroups  $G_e$  of index 2 in  $G$  is to pick a set of generators for  $G$  and consider all combinations in which each generator of *even* order is associated once with  $\epsilon$  (i.e., is in  $G_e$ ) and once with  $\gamma$  (i.e., is not in  $G_e$ ). The resulting black and white point groups then need to be checked for equivalence under arbitrary rotations in  $O(3)$  as explained in Sec. III.B.

As an example, consider the orthorhombic point group  $mm2$ . Taking the two mirrors as generators, one can associate  $\gamma$  with just one of them (in which case the twofold rotation is also associated with  $\gamma$ ) or with both of them. This gives three black and white point groups,  $m'm2'$ ,  $mm'2'$ , and  $m'm'2$ , of which the first two are equivalent through a fourfold rotation which exchanges the two mirrors, yielding just two black and white geometric crystal classes.

#### b. Color arithmetic crystal classes

In practice, what one needs to consider here are the distinct ways of orienting the black and white point group  $G_C$  relative to the lattice  $L$ , as explained in Sec. III.C. As an example, consider the same orthorhombic point group  $mm2$  on a periodic orthorhombic  $C$ -centered lattice. In such a lattice the  $z$  direction is distinguished from the  $x$  and  $y$  directions. The different black and white arithmetic crystal classes (with primes denoting point-group elements associated with  $\gamma$ ) are  $Cm'm2'$  (which is equivalent to  $Cmm'2'$ ),  $Cm'm'2$ ,

$C2'm'm$ ,  $C2'mm'$ , and  $C2m'm'$  (the last three are more commonly expressed in an  $A$  setting as  $Amm'2'$ ,  $Am'm2'$ , and  $Am'm'2$ ). These five classes correspond to the two arithmetic crystal classes  $Cmm2$  and  $C2mm$  in the uncolored case, with the additional distinction between primed and unprimed mirrors.

*c. Color space-group types*

Because there is just one element in  $G_C$  for every element of  $G$ , there is also only one phase function associated with every element of  $G$ . Consequently the group compatibility conditions (11) and their solutions are identical to those one would get when enumerating ordinary (uncolored) space groups, using the standard Fourier-space approach for scalar density functions. Due to the form of the gauge transformation (17), the organization of sets of phase functions, satisfying the group compatibility conditions, into gauge-equivalence classes is also identical to that in the scalar case. Thus, in enumerating black and white space-group types with  $\Gamma_e = \{\epsilon\}$ , one can use the known gauge-equivalence classes of phase functions for the corresponding arithmetic crystal class from the scalar case.

One can specify the black and white space groups in any of the following ways: (1) by taking the international (Hermann-Mauguin) symbol for the corresponding uncolored space group and adding primes to account for the exchange of black and white; (2) by explicitly specifying the lattice  $L$ , the black and white point group  $G_C$ , and the values of the phase functions; or (3) by specifying the group-subgroup pair  $\mathcal{G}(\mathcal{H})$ , where  $\mathcal{G}$  is the space group of the color-blind density and  $\mathcal{H}$  is the space group of one of the components of the color field.

When checking for scale equivalence one needs to be careful to distinguish rotations that are combined with the exchange of black and white from those that are not. This is because no scale transformation (18) can take a phase function of the form  $\Phi_g^\gamma$  into one of the form  $\Phi_g^\epsilon$ . As an example, consider the orthorhombic color arithmetic crystal class  $Cm'm2'$ . Solutions to the group compatibility conditions (which are the same for the colored and uncolored cases) are arranged into four gauge-equivalence classes:  $Cmm2$ ,  $Ccm2_1$ ,  $Cmc2_1$ , and  $Ccc2$ . In the uncolored case,  $Ccm2_1$  and  $Cmc2_1$  are scale equivalent (through the fourfold rotation which exchanges the two mirrors), yielding a total of three space-group types. In the colored case, where only one of the mirrors is primed,  $Cc'm2'_1$  and  $Cm'c2'_1$  are not scale-equivalent, giving a total of four black and white space-group types.

2. The colors are indistinguishable ( $\Gamma = \Gamma_e = \{\epsilon, \gamma\}$ ;  
 $\Gamma/\Gamma_e \approx \mathbb{Z}_2$ )

Because  $\Gamma_e = \Gamma$  every operation  $g$  in  $G$  is associated with both  $\epsilon$  and  $\gamma$ , so there is exactly one black and white point group  $G_C$  for every point group  $G$ . The enumeration of colored geometric and arithmetic crystal

classes is therefore the same as in the uncolored case. The corresponding phase functions—two for every element of  $G$ —satisfy

$$\forall g \in G: \quad \Phi_g^\gamma(\mathbf{k}) \equiv \Phi_g^\epsilon(\mathbf{k}) + \Phi_g^\gamma(\mathbf{k}). \tag{38}$$

Solving the group compatibility conditions (11) associated with the phase functions  $\Phi_g^\epsilon$  and arranging the solutions into gauge-equivalence classes is again identical to solving for the phase functions  $\Phi_g$  when there are no colors. It is thus only necessary to find the (gauge-invariant) phase function  $\Phi_g^\gamma$  and this will determine all the phase functions  $\Phi_g^\gamma$  through Eq. (38) for each of the gauge-equivalence classes. One is then left only with the task of checking for scale equivalence.

Finding the possible solutions for  $\Phi_g^\gamma(\mathbf{k})$  amounts, as explained earlier, to finding all the sublattices  $L_0$  of  $L$  of index 2 that are invariant under the point group  $G$ . Recall that this is equivalent, in the traditional theory of color symmetry, to the task of finding the possible Bravais classes of black and white lattices. The possible solutions for  $\Phi_g^\gamma(\mathbf{k})$  are restricted by the following constraints:

- (1) Since  $\gamma^2 = \epsilon$ , the group compatibility condition (21) requires that

$$\Phi_g^\gamma(\mathbf{k}) \equiv 0 \text{ or } \frac{1}{2}. \tag{39}$$

This corresponds to the assignment of either of the two one-dimensional representations of  $\Gamma_e \approx \mathbb{Z}_2$  to each wave vector  $\mathbf{k}$ . Note that, for any chosen set of lattice generating vectors, at least one must have the value  $\frac{1}{2}$  assigned to it, otherwise all lattice vectors will belong to  $L_0$ .

- (2) Since  $\Gamma$  is Abelian, the requirement (27) that  $\Phi_g^\gamma(\mathbf{k})$  be invariant under the color point group reduces to

$$\forall g \in G: \quad \Phi_g^\gamma(g\mathbf{k}) \equiv \Phi_g^\gamma(\mathbf{k}). \tag{40}$$

The value of  $\Phi_g^\gamma$  is therefore the same on all the vectors in a single orbit or star of the point group  $G$ .

Notation for black and white space groups with  $\Gamma_e = \{\epsilon, \gamma\}$  consists of adding a subscript to the Bravais class symbol indicating the type of sublattice  $L_0$ . The point-group elements are left as in the scalar case (with no primes) with the understanding that each of them appears in the black and white point group both with and without the exchange of black and white.

**B. Axial black and white space groups (on standard lattices)**

Rokhsar, Wright, and Mermin (1988a) have enumerated the two-dimensional axial space-group types on

TABLE II. Two-dimensional axial black and white space-group types. The space groups are given by their International (Hermann-Mauguin) symbol as explained in Sec. V.A, where a prime denotes point-group operations that are combined with the exchange of black and white. The third column lists the black and white space-group types with  $\Gamma_e = \{\epsilon\}$ , describing crystals in which the densities of the two colors are distinguishable. The fourth column lists the black and white space-group types with  $\Gamma_e = \{\epsilon, \gamma\}$ , describing crystals in which the densities of the two colors are indistinguishable. The latter are possible only if the rotational symmetry  $n$  is a power of 2. A subscript  $P$  is added to the Bravais class symbol to indicate the existence of a sublattice  $L_0$  of index 2 in  $L$  describing the color-blind density.

Point-group order $n$	Lattice order $N$	Space groups with $\Gamma_e = \{\epsilon\}$	Space groups with $\Gamma_e = \{\epsilon, \gamma\}$	Periodic example
$n = 2^j, j > 1$	$N = n$	$Pn'$	$P_{pn}$	4
		$\left\{ \begin{array}{l} Pnm'm' \\ Pn'mm' \\ Pn'm'm \end{array} \right.$ $\left\{ \begin{array}{l} Png'm' \\ Pn'gm' \\ Pn'g'm \end{array} \right.$	$P_{pnmm}$  $P_{pn gm}$	
other even $n$	$N = n$	$Pn'$	none	6
		$\left\{ \begin{array}{l} Pnm'm' \\ Pn'mm' \\ Pn'm'm \end{array} \right.$		
$n = p^j, p$ odd prime	$N = 2n$	$Pnm'1$ $Pn1m'$	none	3
other odd $n$	$N = 2n$	$Pnm'$	none	none

standard lattices.<sup>8</sup> Rabson, Mermin, Rokhsar, and Wright (1991, henceforth RMRW) have enumerated the corresponding three-dimensional axial space-group types. We shall use these results to enumerate the black and white axial space-group types in two and three dimensions as outlined in the previous subsection.

The results in two dimensions are given explicitly in Table II. We give a prescription for constructing the three-dimensional black and white space groups by combining the information given in Tables III and IV below and the tables of the ordinary space groups given by RMRW.

1. The colors are distinguishable ( $\Gamma = \{\epsilon, \gamma\}$ ;  $\Gamma_e = \{\epsilon\}$ ;  $\Gamma/\Gamma_e \simeq \mathbb{Z}_2$ )

#### a. Two-dimensional case

The two-dimensional black and white axial space-group types with  $\Gamma_e = \{\epsilon\}$  are listed explicitly by their

international symbol in the third column of Table II. Black and white space groups that correspond to the same uncolored space-group type are grouped together.

#### b. Three-dimensional case

The three-dimensional axial black and white point groups are listed in Table III. These groups are specified in three equivalent ways: by their international symbol, by a set of generating pairs  $(g, \gamma)$ , and by the subgroup  $G_\epsilon$  of  $G$ . Black and white point groups  $G_C$  with the same point group  $G$  are arranged together. This list may be used in conjunction with the tables of RMRW to construct all the three-dimensional axial black and white space-group types on standard lattices. The only intermediate step required is the enumeration of color arithmetic crystal classes. These may be inferred directly from Table III with the following provisos:

- (1) A black and white group, listed in brackets, belongs to the same color geometric crystal class as the group directly above it. When combined with an  $n$ -fold lattice this geometric crystal class results in two different color arithmetic crystal classes, given by the symbols shown.
- (2) As in the uncolored case, when  $n$  is a power of an odd prime the two black and white point groups  $nm'$  and  $n2'$ , when combined with a  $P$  (vertical)

<sup>8</sup>A standard two-dimensional lattice with  $N$ -fold symmetry is composed of all integral linear combinations of an  $N$ -fold star of wave vectors, separated by an angle of  $2\pi/N$ . Mermin, Rokhsar, and Wright (1987) have shown that all  $N$ -fold lattices with  $2 < N < 46$  or  $N = 48, 50, 54, 60, 66, 70, 84,$  and  $90$  are standard. For other values of  $N$  additional types of lattices exist which we do not consider here.

TABLE III. Three-dimensional axial black and white point groups with  $\Gamma_e = \{\epsilon\}$ . The first two columns give the point group  $G$  by listing its international symbol and its generators, where, following the notation of Rabson *et al.* (1991),  $r$  is an  $n$ -fold rotation,  $\bar{r}$  is the same rotation followed by the inversion,  $m$  is a vertical mirror containing the  $n$ -fold rotation axis,  $h$  is a horizontal mirror perpendicular to the  $n$ -fold axis, and  $d$  is a dihedral (twofold) axis perpendicular to the  $n$ -fold axis. The last three columns give the corresponding black and white point groups  $G_C$  in three different ways: (a) by listing their symbol, where primes denote operations that are applied along with the exchange of the two colors; (b) by listing their generators, where  $\gamma$  denotes the exchange of black and white; and (c) by listing the subgroup  $G_\epsilon$ . The information given in this table may be used in conjunction with the tables of Rabson *et al.* (1991) to construct the corresponding list of black and white space-group types, with the following provisos: (1) Black and white point groups in brackets belong to the same color geometric crystal class as the ones above. When used to construct black and white space groups they must be considered in their two orientations relative to the lattice-generating vectors, which produce two distinct color arithmetic crystal classes, given by the two symbols as shown. (2) If  $n$  is a power of an odd prime, the two black and white point groups  $nm'$  and  $n2'$ , when combined with a  $P$  (vertical) lattice, each result in two different color arithmetic crystal classes denoted by  $Pnm'1$ ,  $Pn1m'$ , and  $Pn2'1$ ,  $Pn12'$ .

Point group $G$		Black and white point group $G_C$			
Symbol	Generators	Symbol	Generators	Subgroup $G_\epsilon$	
$\bar{n}$	$\bar{r}$	$\bar{n}'$	$(\bar{r}, \gamma)$	$\frac{n}{2} (n)$	$n$ even (odd)
$\bar{n}2m$ ( $n$ even)	$\bar{r}, m$	$\bar{n}2'm'$	$(\bar{r}, \epsilon), (m, \gamma)$	$\bar{n}$	
		$\bar{n}'2'm$	$(\bar{r}, \gamma), (m, \epsilon)$	$\frac{n}{2} mm \left(\frac{n}{2} m\right)$	$\frac{n}{2}$ even (odd)
		$\bar{n}'2m'$	$(\bar{r}, \gamma), (m, \gamma)$	$\frac{n}{2} 22 \left(\frac{n}{2} 2\right)$	$\frac{n}{2}$ even (odd)
$\bar{n}m$ ( $n$ odd)	$\bar{r}, m$	$\bar{n}m'$	$(\bar{r}, \epsilon), (m, \gamma)$	$\bar{n}$	
		$\bar{n}'m$	$(\bar{r}, \gamma), (m, \epsilon)$	$nm$	
		$\bar{n}'m'$	$(\bar{r}, \gamma), (m, \gamma)$	$n2$	
$n$ ( $n$ even)	$r$	$n'$	$(r, \gamma)$	$\frac{n}{2}$	
$mmm$ ( $n$ even)	$r, m$	$nm'm'$	$(r, \epsilon), (m, \gamma)$	$n$	
		$n'mm'$	$(r, \gamma), (m, \epsilon)$	$\frac{n}{2} mm \left(\frac{n}{2} m\right)$	$\frac{n}{2}$ even (odd)
		$[n'm'm]$	$[(r, \gamma), (m, \gamma)]$		$["]$
$nm$ ( $n$ odd)	$r, m$	$nm'$	$(r, \epsilon), (m, \gamma)$	$n$	
$n22$ ( $n$ even)	$r, d$	$n2'2'$	$(r, \epsilon), (d, \gamma)$	$n$	
		$n'22'$	$(r, \gamma), (d, \epsilon)$	$\frac{n}{2} 22 \left(\frac{n}{2} 2\right)$	$\frac{n}{2}$ even (odd)
		$[n'2'2]$	$[(r, \gamma), (d, \gamma)]$		$["]$
$n2$ ( $n$ odd)	$r, d$	$n2'$	$(r, \epsilon), (d, \gamma)$	$n$	
$n/m$ ( $n$ even)	$r, h$	$n/m'$	$(r, \epsilon), (h, \gamma)$	$n$	
		$n'/m$	$(r, \gamma), (h, \epsilon)$	$\frac{n}{2} / m (\bar{n})$	$\frac{n}{2}$ even (odd)
		$n'/m'$	$(r, \gamma), (h, \gamma)$	$\bar{n} \left(\frac{\bar{n}}{2}\right)$	$\frac{n}{2}$ even (odd)

TABLE III. (Continued).

Point group $G$		Black and white point group $G_C$			
Symbol	Generators	Symbol	Generators	Subgroup $G_\epsilon$	
$n/mmm$ ( $n$ even)	$r, h, m$	$n/m'mm$	$(r, \epsilon), (h, \gamma), (m, \epsilon)$	$nmm$	
		$n/mm'm'$	$(r, \epsilon), (h, \epsilon), (m, \gamma)$	$n/m$	
		$n/m'm'm'$	$(r, \epsilon), (h, \gamma), (m, \gamma)$	$n22$	
		$n'/mmm'$	$(r, \gamma), (h, \epsilon), (m, \epsilon)$	$\frac{n}{2} / mmm (\bar{n}2m)$	$\frac{n}{2}$ even (odd)
		$[n'/mm'm]$	$[(r, \gamma), (h, \epsilon), (m, \gamma)]$		$[']$
		$n'/m'mm'$	$(r, \gamma), (h, \gamma), (m, \epsilon)$	$n\bar{2}m \left(\frac{\bar{n}}{2}m\right)$	$\frac{n}{2}$ even (odd)
		$[n'/m'm'm]$	$[(r, \gamma), (h, \gamma), (m, \gamma)]$		$[']$

lattice, each result in two different color arithmetic crystal classes denoted by  $Pnm'1$ ,  $Pn1m'$ , and  $Pn2'1$ ,  $Pn12'$ .

As an example, let us use Table III to construct the list of black and white space-group types with point group  $10/mmm$ . There are four gauge-equivalence classes of solutions to the group compatibility conditions leading, in the scalar case, to four distinct space-group types denoted by  $P10/mmm$ ,  $P10/mcc$ ,  $P10_5/mmc$ , and  $P10_5/mcm$  (see Table XI of RMRW). The same solutions exist for the black and white space groups, only now we need to consider for each of the four solutions the seven different ways of associating  $\epsilon$  and  $\gamma$  with the elements of the point group as shown at the bottom of Table III. This gives a total of 28 black and white space-group types associated with the point group  $10/mmm$ . The seven black and white space-group types corresponding to the second solution, for example, would be denoted by  $P10/m'cc$ ,  $P10/mc'c'$ ,  $P10/m'c'c'$ ,  $P10'/mcc'$ ,  $P10'/mc'c$ ,  $P10'/m'cc'$ , and  $P10'/m'c'c$ .

2. The colors are indistinguishable ( $\Gamma = \Gamma_\epsilon = \{\epsilon, \gamma\}$ ;  
 $\Gamma/\Gamma_\epsilon \cong \mathbb{Z}_2$ )

#### a. Two-dimensional case

A standard two-dimensional  $N$ -fold lattice  $L$  may be generated by an  $N$ -fold star of wave vectors, denoted here by  $\mathbf{b}_1 \dots \mathbf{b}_N$  where  $N$  is even. We want to find all distinct sublattices  $L_0$  of index 2 in  $L$  that are invariant under the point group  $G$ . This amounts to finding the possible values for the phase function  $\Phi_\epsilon^\gamma$  that satisfy the group compatibility conditions and, if applicable, checking for scale equivalence among them.

From the general considerations outlined earlier, summarized by Eqs. (39) and (40), all the vectors in the  $N$ -fold star have the same phase  $\Phi_\epsilon^\gamma(\mathbf{b}_i)$ , which is either 0 or  $\frac{1}{2}$ . If  $p$  is a divisor of  $N$  then there is a  $p$ -fold star of wave vectors among the  $\mathbf{b}_i$  which add up to zero. The linearity of the phase function then requires that  $p\Phi_\epsilon^\gamma(\mathbf{b}_i) \equiv 0$ , which for odd  $p$  implies that  $\Phi_\epsilon^\gamma(\mathbf{b}_i) \equiv 0$ . Thus the phase associated with the vectors of the  $N$ -fold star can be  $\frac{1}{2}$  only if  $N$  is a power of 2. As a consequence,

a standard  $N$ -fold lattice may have an invariant sublattice of index 2 only if  $N$  is a power of 2.

Since there is only one solution, one does not need to check for scale equivalence. The resulting black and white space-group types, one for each uncolored space-group type, are listed in the fourth column of Table II. A subscript  $P$  denotes the fact that the lattice of the color-blind density  $L_0$  is a sublattice of  $L$  that is also a standard  $N$ -fold lattice.

#### b. Three-dimensional case

Let us first review the different Bravais classes of standard axial lattices in three dimensions.<sup>9</sup> All such lattices are constructed by stacking two-dimensional standard lattices in the third dimension. It is always possible to construct three-dimensional axial lattices by adding to the  $N$ -fold generating star of the horizontal sublattice a vertical stacking vector  $\mathbf{c}$  along the axis of rotation. The rotational symmetry of the vertically stacked lattice is the same rotational symmetry  $N$  of its horizontal sublattice, which is always even. The Bravais class of such lattices is denoted either by a  $V$  (for "vertical") or by a  $P$  (for "primitive").

Only if  $N$  is twice a power of a single prime is it also possible to have a second Bravais class, in which the horizontal sublattices are stacked by a staggered stacking vector  $\mathbf{c}_s = \mathbf{c} + \mathbf{h}$  with a horizontal shift  $\mathbf{h}$  from layer to layer. When  $N$  is a power of 2, the staggered lattice continues to have the full  $N$ -fold symmetry; when  $N$  is twice an odd prime the rotational symmetry  $n$  of the staggered lattice is half that of its horizontal sublattice. The Bravais class of staggered lattices is denoted by  $S$  (for "staggered") except for the trigonal and tetragonal cases, where the more common notation is  $R$  (for "rhombohedral") and  $I$  (for "body-centered"). We note that a staggered lattice with  $n$ -fold symmetry ( $n = p^s$ ,  $p$  prime) repeats every  $p$  layers. Furthermore, we note that the staggered stacking vector  $\mathbf{c}_s$  may always be cho-

<sup>9</sup>For more detail see Mermin, Rabson, Rokhsar, and Wright (1990) or the summary in RMRW (Rabson *et al.*, 1991).

TABLE IV. Invariant sublattices of index 2 in standard three-dimensional axial lattices. The sublattices are found by solving the group compatibility conditions for the phase function  $\Phi_e^\gamma$  as detailed in Sec. V.B.2. The solutions are given by the values of the phase function at the vectors  $\mathbf{b}_i$  which generate the horizontal sublattice and at the additional stacking vector,  $\mathbf{c}$  in the vertical case, and  $\mathbf{c}_s$  in the staggered case. The solutions, previously derived in five-dimensional superspace by Niizeki (1990b) for the special cases  $n=5,8,10,12$ , agree with the results given here. A subscript is added to the Bravais class symbol of  $L$  to indicate the type of sublattice  $L_0$ , as explained in Sec. V.B.2. These symbols may be directly combined with the symbols of the uncolored space-group types, given Rabson *et al.* (1991), to produce the corresponding axial black and white space-group types. For example, the uncolored space group  $P10/mcc$  produces one black and white space-group type,  $P_{2c}10/mcc$ , whereas the space group  $P8/mcc$  gives three black and white space-group types:  $P_{2c}8/mcc$ ,  $P_p8/mcc$ , and  $P_s8/mcc$ .

Point group order $n$	Vertical stacking		Staggered stacking		Periodic example
	$\Phi_e^\gamma(\mathbf{b}_i)$	$\Phi_e^\gamma(\mathbf{c})$	$\Phi_e^\gamma(\mathbf{b}_i)$	$\Phi_e^\gamma(\mathbf{c}_s)$	
$n=2^j, j>1$	$P_{2c}$ : 0	$\frac{1}{2}$	$S_p$ : 0	$\frac{1}{2}$	4
	$P_p$ : $\frac{1}{2}$	0			
	$P_s$ : $\frac{1}{2}$	$\frac{1}{2}$			
other even $n$	$P_{2c}$ : 0	$\frac{1}{2}$	N/A		6
$n=p^j, p$ odd prime	$P_{2c}$ : 0	$\frac{1}{2}$	$S_s$ : 0	$\frac{1}{2}$	3
other odd $n$	$P_{2c}$ : 0	$\frac{1}{2}$	N/A		none

sen such that when subtracted from its image under an  $n$ -fold rotation  $r_n$  gives one of the vectors in the  $N$ -fold horizontal star:

$$r_n \mathbf{c}_s - \mathbf{c}_s = \mathbf{b}_i. \tag{41}$$

We know from the two-dimensional analysis above that the possible phases associated with the vectors of the  $N$ -fold star (before considering stacking) are

$$\Phi_e^\gamma(\mathbf{b}_i) \equiv \begin{cases} 0 \text{ or } \frac{1}{2} & N=2^s, \\ 0 & N \neq 2^s. \end{cases} \tag{42}$$

The vertical stacking vector  $\mathbf{c}$  is independent of the generators of the horizontal sublattice, so the phase  $\Phi_e^\gamma(\mathbf{c})$  may independently be zero or  $\frac{1}{2}$ . This gives for vertical lattices a total of three solutions when  $N$  is a power of 2 and a single solution otherwise, as summarized in the second column of Table IV. We denote by  $P_{2c}$  the solution in which only the stacking vector  $\mathbf{c}$  has a phase value of  $\frac{1}{2}$  to indicate that the sublattice  $L_0$  of the color-blind density contains all the even layers of  $L$ . The symbol  $P_p$  denotes the solution in which only the horizontal generating vectors  $\mathbf{b}_i$  are given the value  $\frac{1}{2}$ . The sublattice  $L_0$  in this case is also a  $P$  lattice with the same periodic spacing as  $L$ . The third solution in which all the generating vectors are assigned the value  $\frac{1}{2}$  is denoted by  $P_s$  because in this case the sublattice  $L_0$  is staggered.

The staggered stacking vector  $\mathbf{c}_s$  is not independent of the  $\mathbf{b}_i$ . The phase  $\Phi_e^\gamma(\mathbf{c}_s)$  may be 0 or  $\frac{1}{2}$ , but the linear constraint of Eq. (41) implies that in the case of staggered lattices the phases at the  $N$ -fold horizontal star must be zero because from Eq. (40)

$$\Phi_e^\gamma(\mathbf{b}_i) \equiv \Phi_e^\gamma(r_n \mathbf{c}_s) - \Phi_e^\gamma(\mathbf{c}_s) \equiv 0. \tag{43}$$

This gives only one solution for staggered lattices, summarized in the third column of Table IV. We denote this solution by  $S_s$  if  $N=2p^s$  and  $p$  is an odd prime, and by  $S_p$  if  $p=2$ . This is because horizontal sublattices repeat

every  $p$  layers, yielding a vertical sublattice  $L_0$  if  $p=2$  and a staggered one otherwise.

The results, previously derived by Niizeki (1990b) for the special case of rank-5 axial lattices ( $n$ -fold lattices with  $n=5,8,10,12$ ), agree with our general results shown in Table IV. To construct a list of all the black and white space-group types (with black and white in the same indistinguishability class) one simply has to prepend to the symbol of each uncolored space-group type the symbols from Table IV denoting the possible solutions for  $\Phi_e^\gamma$ . In this way, for example, the uncolored space group  $P10/mcc$  produces one black and white space-group type,  $P_{2c}10/mcc$ , whereas the space group  $P8/mcc$  gives three black and white space-group types:  $P_{2c}8/mcc$ ,  $P_p8/mcc$ , and  $P_s8/mcc$ .

### C. Icosahedral black and white space groups

We conclude this section by enumerating the icosahedral black and white space-group types. The results of the enumeration are given in two tables: Table V lists the black and white space-group types with  $\Gamma_e = \{\epsilon\}$  where the two colors belong to two indistinguishability classes of colors; Table VI lists the space-group types with  $\Gamma_e = \{\epsilon, \gamma\}$  where the two colors belong to a single indistinguishability class.

1. The colors are distinguishable ( $\Gamma = \{\epsilon, \gamma\}$ ;  $\Gamma_e = \{\epsilon\}$ ;  $\Gamma/\Gamma_e \cong Z_2$ )

The space groups with  $\Gamma_e = \{\epsilon\}$  are very simple because in this case there is only one black and white icosahedral point group. It is associated with the full icosahedral point group  $\bar{5}\bar{3}\bar{m}$  and its proper subgroup 532, which is of index 2. The exchange of black and white is associated with all the improper rotations. The black and white point group is therefore denoted by  $\bar{5}'\bar{3}'m'$ . The black and white icosahedral space groups

TABLE V. Icosahedral black and white space-group types with  $\Gamma_e = \{\epsilon\}$ . The black and white point group associates the exchange of the two colors with all the improper rotations of the full icosahedral group, as denoted by primes in the space-group symbol. It may be generated by the two elements  $(m, \gamma)$  and  $(\bar{r}_3, \gamma)$ . Their associated phase functions are taken from those of the corresponding generators  $m$  and  $\bar{r}_3$  in the uncolored case. The phase function  $\Phi_m^\gamma$  is given by its values on the sets of generators for the icosahedral lattices used by Mermin (1992, see p. 18). The phase function  $\Phi_{\bar{r}_3}^\gamma$  is zero everywhere in an appropriate gauge. The space-group types are also given in terms of a group-subgroup pair  $\mathcal{G}(\mathcal{H})$ , in which  $\mathcal{G}$  is the space group of the color-blind density and  $\mathcal{H}$  is the space group describing the symmetry of one of the colors. There is a slight discrepancy with the results previously derived by Sheng (1994, Table 3.3.)

	$\bar{5}\bar{3}\frac{2}{m}(Y_h)$	$\Phi_m^\gamma$	$\mathcal{G}(\mathcal{H})$
$P$	$P\bar{5}\bar{3}'\frac{2}{m'}$	000 000	$P\bar{5}\bar{3}\frac{2}{m}$ ( $P532$ )
	$P\bar{5}\bar{3}'\frac{2}{q'}$	$\frac{1}{2}\frac{1}{2}0$ 000	$P\bar{5}\bar{3}\frac{2}{q}$ ( $P532$ )
$F^*(I)$	$F^*\bar{5}\bar{3}'\frac{2}{m'}$	000 000	$F^*\bar{5}\bar{3}\frac{2}{m}$ ( $F^*532$ )
$I^*(F)$	$I^*\bar{5}\bar{3}'\frac{2}{m'}$	000 000	$I^*\bar{5}\bar{3}\frac{2}{m}$ ( $I^*532$ )
	$I^*\bar{5}\bar{3}'\frac{2}{q'}$	$\frac{1}{2}\frac{1}{2}0$ $00\frac{1}{2}$	$I^*\bar{5}\bar{3}\frac{2}{q}$ ( $I^*532$ )

with  $\Gamma_e = \{\epsilon\}$  are listed in Table V. They follow directly from the uncolored space-group types, tabulated by Mermin (1992, Table VIII).

2. The colors are indistinguishable ( $\Gamma = \Gamma_e = \{\epsilon, \gamma\}$ ;  
 $\Gamma/\Gamma_e \cong Z_4$ )

For the enumeration of the icosahedral black and white space-group types with  $\Gamma_e = \{\epsilon, \gamma\}$  we need to find the distinct solutions for the phase function  $\Phi_e^\gamma(\mathbf{k})$ . There are three Bravais classes of rank-6 icosahedral lattices:<sup>10</sup>  $P$  (primitive),  $F^*$  (face centered in Fourier space), and  $I^*$  (body centered in Fourier space). We shall consider each one separately.

a. Primitive icosahedral lattices

An icosahedral  $P$  lattice can be generated by taking all integral linear combinations of a single star of 12 wave vectors pointing to the vertices of an icosahedron (only 6 of the 12 vectors are integrally independent). The value of the phase function  $\Phi_e^\gamma$  must be the same on all the 12 vectors of the star. We need to check whether there are any linear relations among these wave vectors

<sup>10</sup>For details see Rokhsar, Mermin, and Wright (1987) or Mermin (1992, p. 18)

TABLE VI. Icosahedral black and white space-group types with  $\Gamma_e = \{\epsilon, \gamma\}$ . Such space groups exist only on  $P$  and  $I^*$  lattices. When the point group  $G$  is  $\bar{5}\bar{3}\bar{m}$ , the black and white point group is generated by  $(e, \gamma)$ ,  $(\bar{r}_3, \epsilon)$ , and  $(m, \epsilon)$ . When the point group  $G$  is 532, the black and white point group is generated by  $(e, \gamma)$ ,  $(r_3, \epsilon)$ , and  $(r_2, \epsilon)$ . The possible values of the phase function  $\Phi_e^\gamma$  are derived in the text. The values for the other phase functions are taken from the uncolored case as tabulated by Mermin (1992, Tables VIII and IX). All phase functions are given by their values on the sets of generators for the icosahedral lattices as chosen by Mermin (1992, p. 18). The solution for the phase function  $\Phi_e^\gamma$  is denoted in the space-group symbol by adding a subscript, which specifies the Bravais class of the sublattice  $L_0$  of the color-blind density. The space-group types are also given in terms of a group-subgroup pair  $\mathcal{G}(\mathcal{H})$ , in which  $\mathcal{G}$  is the space group of the color-blind density and  $\mathcal{H}$  is the space group describing the symmetry of one of the colors. There are some discrepancies with the results previously derived by Sheng (1994, Tables 3.4 and 3.5). Note particularly that the nonsymmorphic uncolored space-group type  $I^*\bar{5}\bar{3}\bar{2}/q$  turns into three black and white space-group types, denoted by  $I_p^*\bar{5}\bar{3}\bar{2}/q$ ,  $I_p^*\bar{5}\bar{3}\bar{2}/r$ , and  $I_p^*\bar{5}\bar{3}\bar{2}/s$ ; for these three space-group types the  $\mathcal{G}(\mathcal{H})$  symbol is not unique and should be avoided.

$P$	$\bar{5}\bar{3}\frac{2}{m}(Y_h)$	$\Phi_e^\gamma$	$\Phi_m^\epsilon$	$\mathcal{G}(\mathcal{H})$
	$P_{F^*}\bar{5}\bar{3}\frac{2}{m}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	000 000	$F^*\bar{5}\bar{3}\frac{2}{m}$ $\left(P\bar{5}\bar{3}\frac{2}{m}\right)$
	$P_{F^*}\bar{5}\bar{3}\frac{2}{q}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}0$ 000	$F^*\bar{5}\bar{3}\frac{2}{q}$ $\left(P\bar{5}\bar{3}\frac{2}{q}\right)$
	532 ( $Y$ )	$\Phi_e^\gamma$	$\Phi_{r_2}^\epsilon$	$\mathcal{G}(\mathcal{H})$
	$P_{F^*}532$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	000 000	$F^*532$ ( $P532$ )
	$P_{F^*}5_{132}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{5}00$ $\frac{4}{5}\frac{1}{5}0$	$F^*5_{132}$ ( $P5_{132}$ )
$I^*(F)$	$\bar{5}\bar{3}\frac{2}{m}(Y_h)$	$\Phi_e^\gamma$	$\Phi_m^\epsilon$	$\mathcal{G}(\mathcal{H})$
	$I_p^*\bar{5}\bar{3}\frac{2}{m}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ 000	000 000	$P\bar{5}\bar{3}\frac{2}{m}$ $\left(I^*\bar{5}\bar{3}\frac{2}{m}\right)$
	$I_p^*\bar{5}\bar{3}\frac{2}{q}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ 000	$\frac{1}{2}\frac{1}{2}0$ $00\frac{1}{2}$	$P\bar{5}\bar{3}\frac{2}{q}$ $\left(I^*\bar{5}\bar{3}\frac{2}{q}\right)$
	$I_p^*\bar{5}\bar{3}\frac{2}{r}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ 000	$00\frac{1}{2}$ $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$P\bar{5}\bar{3}\frac{2}{q}$ $\left(I^*\bar{5}\bar{3}\frac{2}{q}\right)$
	$I_p^*\bar{5}\bar{3}\frac{2}{s}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ 000	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ $\frac{1}{2}\frac{1}{2}0$	$P\bar{5}\bar{3}\frac{2}{q}$ $\left(I^*\bar{5}\bar{3}\frac{2}{q}\right)$
	532 ( $Y$ )	$\Phi_e^\gamma$	$\Phi_{r_2}^\epsilon$	$\mathcal{G}(\mathcal{H})$
	$I_p^*532$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ 000	000 000	$P532$ ( $I^*532$ )
	$I_p^*5_{132}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ 000	$\frac{1}{5}0\frac{1}{5}\frac{3}{5}0\frac{3}{5}$	$P5_{132}$ ( $I^*5_{132}$ )

which would disallow this value from being  $\frac{1}{2}$ . This can happen only if there is an odd number of vectors in the star that sum to zero. Since this is not the case, the non-trivial solution, assigning the phase function  $\Phi_e^\gamma$  a value of  $\frac{1}{2}$  on the vectors of the star, exists. The color-blind sublattice is an  $F^*$  lattice, generated by taking integral

linear combinations containing an even number of the 12 vectors from the original star.

*b. Face-centered icosahedral lattices*

An icosahedral  $F^*$  lattice can be generated by a single star of 30 wave vectors pointing to the midpoints along the edges of an icosahedron (along the twofold axes). Because the twofold axes are perpendicular to threefold axes there exist many triplets among the 30 vectors of the star that sum to zero. For this reason it is not possible to assign the phase function  $\Phi_e^\gamma$  a value of  $\frac{1}{2}$  on the vectors of the star. Consequently an icosahedral  $F^*$  lattice has no icosahedral sublattice of index 2 and therefore there cannot be black and white space groups on  $F^*$  lattices where the two colors are indistinguishable.

*c. Body-centered icosahedral lattices*

An icosahedral  $I^*$  lattice can be generated by two concentric stars, of 12 vectors each, pointing to the vertices of an icosahedron, with one star a factor  $\tau$  larger than the other ( $\tau$  being the golden mean). On each star we can independently set the value of the phase function  $\Phi_e^\gamma$  to zero or  $\frac{1}{2}$ , because each star by itself is the same as the single star that generates a  $P$  lattice, and any combination of vectors that sum to zero contains an even number of vectors from each star. The three nontrivial solutions, setting the value of  $\Phi_e^\gamma$  to  $\frac{1}{2}$  on the inner star, on the outer star, or on both, are scale-equivalent under successive rescaling of the lattice by a factor of  $\tau$  and therefore produce only one distinct solution. The color-blind lattice is a  $P$  lattice generated either by the 12 vectors of the outer star, the 12 vectors of the inner star, or the 12 vectors of a third star a factor  $\tau^2$  larger than the inner star.

These results agree with those found by Niizeki (1990a) for the black and white icosahedral lattices in six-dimensional superspace. To generate the list of black and white space-group types we take the solutions for the gauge-equivalence classes in the uncolored case, which were tabulated by Mermin (1992, Tables VIII and IX), and use them for the phase functions  $\Phi_e^\epsilon$ . As a notation for the black and white space group we take the corresponding notation for the uncolored space group and add a subscript to the Bravais class symbol which specifies the Bravais class of the color-blind sublattice. In the case of the  $I^*$  Bravais class some care is needed when checking for scale equivalence, since scale equivalence is also used to relate the three solutions for  $\Phi_e^\gamma$ . When the point group is  $\bar{5}3m$  we find that three gauge-equivalence classes that were scale-equivalent in the uncolored case are no longer scale-equivalent in the black and white case and give rise to three distinct black and white space-group types, which differ in their glide planes. When the point group is  $532$  we find that the gauge-equivalence classes that are scale-equivalent in the uncolored case remain scale-equivalent in the black and white case as well. These results are summarized in Table VI.

## VI. LATTICE COLOR GROUPS OF STANDARD TWO-DIMENSIONAL AXIAL LATTICES

An important step in enumerating the color space-group types for lattices  $L$  in a given Bravais class is to find the possible lattice color groups  $\Gamma_e$  that are compatible with  $L$ . In this section we shall use a very simple geometric approach, which will yield a partial answer to this question, namely, the possible orders of lattice color groups  $\Gamma_e$  that are compatible with  $L$ . We shall be looking for the possible indices of invariant sublattices  $L_0$  of  $L$ , which due to the isomorphism between  $L/L_0$  and  $\Gamma_e$  determine the number of elements in  $\Gamma_e$ .

In the special case when all the colors belong to a single indistinguishability class the lattice color group  $\Gamma_e$ , which is Abelian, is also required to be transitive on all the colors. One can easily show that under such circumstances the order of  $\Gamma_e$  is equal to the total number of colors.<sup>11</sup> Thus finding the possible indices of invariant sublattices  $L_0$  of  $L$  also enables one to determine the possible numbers  $n$  of colors in color fields with lattice  $L$  in which all the components of the field are indistinguishable. In the previous section we fixed the number of colors to  $n=2$  and looked for the possible lattices  $L$  that could accommodate a two component color field in which the components are indistinguishable. Here we fix  $L$  and look for the possible numbers  $n$  of colors.

The geometric procedure that we use here is very similar to the one used by Harker (1978b) to enumerate “colored lattices” in the periodic case. A different approach to this question, which involves the use of generating functions of Dirichlet series, is taken by Baake (1997). Baake’s algebraic approach gives the possible indices of invariant sublattices and also the number of distinct sublattices with a given index. We determine the actual distinct sublattices of a given index either by solving the group compatibility conditions (21) on the phase functions  $\Phi_e^\gamma(\mathbf{k})$ , as we did in Sec. V in the case of black and white groups, or equivalently, by considering the distinct modular lattices  $L/L_0$  compatible with the required symmetry, as we shall do in Sec. VII when we enumerate the pentagonal and decagonal color space-group types.

We shall consider here the case of two-dimensional  $N$ -fold lattices, with  $2 < N < 46$ .  $N$  is necessarily even because any lattice contains the negative of its vectors. Mermin, Rokhsar, and Wright (1987) have shown that all such lattices are *standard*—they consist of all integral linear combinations of an  $N$ -fold star of wave vectors, separated by an angle of  $2\pi/N$ . Consequently any invariant sublattice of such a standard  $N$ -fold lattice must itself be a standard  $N$ -fold lattice.

Any arbitrary vector  $\mathbf{h} \in L$  belongs to an  $N$ -fold star which generates a sublattice  $L_0$  of  $L$ . One can thus generate all the sublattices of  $L$  simply by letting  $\mathbf{h}$  run

<sup>11</sup>A permutation group that is transitive on  $n$  colors clearly contains at least  $n$  elements. One can easily show that if it contains more than  $n$  elements it cannot be Abelian.

through all wave vectors in  $L$ . The index of the sublattice may be calculated by taking the magnitude of the determinant of the matrix, which gives the basis of  $L_0$  in terms of the basis of  $L$ . If one requires the sublattice also to be invariant under the mirrors that leave  $L$  invariant, then the vector  $\mathbf{h}$  must be restricted to lie either along one of the mirrors or exactly between two of them.

The smallest point group to consider on an  $N$ -fold lattice is  $G=n$ , generated by an  $n$ -fold rotation  $r_n$ , where

$$n = \begin{cases} N & N \text{ twice an even integer,} \\ \frac{N}{2} & N \text{ twice an odd integer.} \end{cases} \quad (44)$$

It is convenient<sup>12</sup> to generate the  $N$ -fold lattice  $L$  with the integrally independent subset of star vectors  $\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_D$ , where

$$r_n \mathbf{b}_j = \begin{cases} \mathbf{b}_{j+1} & j=1, \dots, D-1, \\ \sum_{i=1}^D k_i \mathbf{b}_i & j=D. \end{cases} \quad (45)$$

The rank  $D$  of the lattice is given by the Euler totient function  $D = \phi(N)$ , which is defined as the number of positive integers less than and relatively prime to  $N$ , and is calculated by

$$D = \Phi(N) = N \prod_i \frac{p_i - 1}{p_i}, \quad (46)$$

where  $p_i$  are the distinct prime factors of  $N$ . The integral coefficients  $k_i$  in Eq. (45), giving  $r_n \mathbf{b}_D$  in terms of  $\mathbf{b}_1, \dots, \mathbf{b}_D$ , can easily be determined for any given lattice.

With this choice of basis the vector  $\mathbf{h}$  is represented by a column vector  $\vec{H}$ , consisting of  $D$  arbitrary integers, and the  $n$ -fold rotation  $r_n$  is represented by the  $D \times D$  matrix

$$\mathcal{R} = \begin{pmatrix} 0 & \dots & 0 & k_1 \\ 1 & & & k_2 \\ & \ddots & & \vdots \\ & & 1 & k_D \end{pmatrix}. \quad (47)$$

The basis of  $L_0$  is given by  $\vec{H}, \mathcal{R}\vec{H}, \dots, \mathcal{R}^{D-1}\vec{H}$ , and the index of  $L_0$  in  $L$  is simply

$$m = |\det(\vec{H} \quad \mathcal{R}\vec{H} \quad \dots \quad \mathcal{R}^{D-1}\vec{H})|. \quad (48)$$

The index  $m$  is therefore a function of the  $D$  independent integers that determine  $\vec{H}$  and can have no other form than that given by Eq. (48).

For any given standard  $N$ -fold lattice we determine the rank  $D$  and the integers  $k_i$  in Eq. (45). We then use a simple MATHEMATICA program to generate the deter-

minant in Eq. (48) and to calculate its possible values up to a given cutoff. The results for sublattices, invariant under the point group  $G=n$ , are summarized in Table VII for  $N$ -fold lattices up to rank  $D=8$ . In Table VIII we give the restricted values of the indices  $m$  for sublattices that are invariant under the full point group of  $L$  up to rank  $D=4$ .

## VII. DECAGONAL AND PENTAGONAL COLOR SPACE GROUPS IN TWO DIMENSIONS

To illustrate many of the ideas presented in this paper, we conclude with an enumeration of the decagonal and pentagonal color space-group types in two dimensions, explicitly listing them for color fields with up to 25 colors. This example avoids some unnecessary complications owing to the fact that ordinary decagonal and pentagonal space groups for uncolored crystals are all symmorphic—in a suitably chosen gauge all the phase functions are zero everywhere on the lattice.<sup>13</sup>

The lattice  $L$ , which in this example is the two-dimensional tenfold lattice, contains a fivefold star of vectors (shown in Fig. 6) of which four, labeled  $\mathbf{b}_1 \dots \mathbf{b}_4$ , can be taken as integrally independent lattice-generating vectors. The lattice point group is  $10mm$ , generated by the tenfold rotation  $r_{10}$  and either a mirror of type  $m_1$  which leaves the fivefold star invariant or a mirror of type  $m_2$  which takes the star into the fivefold star containing the negatives of the lattice-generating vectors.

We first determine the abstract structure of the modular lattices  $L/L_0$  and therefore also of lattice color groups  $\Gamma_e$ , compatible with  $L$ . We then explicitly specify the values of the distinct sets of phase functions  $\Phi_e^{\gamma}(\mathbf{k})$  which satisfy the group compatibility conditions (11). We then specify the actual lattice color groups  $\Gamma_e$ , which allows us to proceed to the actual enumeration of color point groups and color space-group types.

### A. Decagonal and pentagonal point groups and their subgroups

When enumerating color space groups on the decagonal lattice, the point group  $G$  of the color field may be taken as the full lattice point group  $10mm$  or any of the following subgroups:  $10$ ,  $5m$  (in its two orientations with respect to the lattice  $5m1$  and  $51m$ ), and  $5$ . For each of these choices of  $G$  we list in Table IX all the possible subgroups  $H$ , the corresponding normal subgroup  $H_0$  (if different from  $H$ ), and the index  $q$  of  $H$  in  $G$ . These values of  $q$  (1, 2, 4, 5, 10, and 20) determine the possible numbers of indistinguishability classes of colors in a two-dimensional decagonal or pentagonal color field. Also listed in Table IX are the indistinguishability-class permutations associated with the generators of  $G$ , which

<sup>12</sup>For a justification of this choice of lattice-generating vectors see, for example, footnote 8 in Rabson *et al.* (1991).

<sup>13</sup>For more detail see Rokhsar, Wright, and Mermin (1988b).

TABLE VII. Possible indices of invariant sublattices of standard two-dimensional  $N$ -fold lattices (without mirror symmetry). The values of these indices are equal to the possible numbers of colors in an  $N$ -fold symmetric color field whose components are all indistinguishable, or equivalently, to the orders of lattice color groups  $\Gamma_e$ , compatible with an  $N$ -fold lattice. The sublattices are required to be invariant only under the point group  $G=n$  and not under the full point group of the  $N$ -fold lattice, which also contains mirror reflections. The indices are calculated by evaluating the determinant in Eq. (48), letting the  $D$  integral components of the arbitrary vector  $\vec{H}$  run between properly chosen values.

Lattice order $N$	Point group $G$	Possible indices of sublattices, invariant under $G=n$
Rank 2		
4	4	1,2,4,5,8,9,10,13,16,17,18,20,25,26,29,32,34,36,37, . . .
6	3,6	1,3,4,7,9,12,13,16,19,21,25,27,28,31,36,37,39,43, . . .
Rank 4		
8	8	1,2,4,8,9,16,17,18,25,32,34,36,41,49,50,64,58,72, . . .
10	5,10	1,5,11,16,25,31,41,55,61,71,80,81,101,121,125,131, . . .
12	12	1,4,9,13,16,25,36,37,49,52,61,64,73,81,97,100,109, . . .
Rank 6		
14	7,14	1,7,8,29,43,49,56,64,71,113,127,169,197,203,211,232, . . .
18	9,18	1,3,9,19,27,37,57,64,73,81,109,111,127,163,171,181, . . .
Rank 8		
16	16	1,2,4,8,16,17,32,34,49,64,68,81,97,113,128,136,162, . . .
20	20	1,5,16,25,41,61,80,81,101,121,125,181,205,241,256, . . .
24	24	1,4,9,16,25,36,49,64,73,81,97,100,121,144,169,193, . . .
30	15,30	1,16,25,31,61,81,121,151,181,211,241,256,271,331, . . .

are uniquely determined by the subgroup  $H$ . The information given in Table IX is illustrated graphically in Fig. 7.

**B. Decagonal modular lattices  $L/L_0$**

For any choice of  $L_0$ , the modular lattice  $L/L_0$  may still be generated by the same four wave vectors  $\mathbf{b}_1 \dots \mathbf{b}_4$  that generate  $L$ , but in general these vectors may no longer be integrally independent modulo  $L_0$ . If the first  $l$  vectors  $\mathbf{b}_1 \dots \mathbf{b}_l$  ( $1 \leq l \leq 4$ ) cannot be expressed as integral linear combinations (modulo  $L_0$ ) of each other and

$$\mathbf{b}_{l+1} = \sum_{i=1}^l h_i \mathbf{b}_i \text{ (modulo } L_0) \tag{49}$$

for some integral coefficients  $h_i$ , then due to the fivefold symmetry of  $L$  and  $L_0$  all other vectors in the fivefold star may be expressed as integral linear combinations (modulo  $L_0$ ) of the first  $l$ . The vectors  $\mathbf{b}_1 \dots \mathbf{b}_l$  can thus be taken as a generating basis for the modular lattice  $L/L_0$ .

If  $m$  is the smallest integer such that  $m\mathbf{b}_1$  is in  $L_0$ , then fivefold symmetry requires  $m$  to satisfy the same condition for the other generators of  $L/L_0$ . Any vector in  $L/L_0$  can therefore be expressed as an integral linear combination of the generators  $\mathbf{b}_1 \dots \mathbf{b}_l$  with coefficients

between 0 and  $m-1$ . The modular lattice  $L/L_0$  is a rank- $l$  lattice in which arithmetic is performed modulo  $m$ .

If the generators  $\mathbf{b}_1 \dots \mathbf{b}_l$  are integrally independent modulo  $L_0$  (i.e.,  $\sum_{i=1}^l c_i \mathbf{b}_i \in L_0$  implies that all  $c_i = 0 \pmod m$ ) then as an Abelian group the modular lattice is isomorphic to  $(\mathbb{Z}_m)^l$ —the direct product of  $l$  cyclic groups, each of order  $m$ . The modular lattice  $L/L_0$  contains  $m^l$  vectors or, equivalently, the index of  $L_0$  in  $L$  is  $m^l$ . Determining the lattice color group  $\Gamma_e$  to within isomorphism amounts to finding the possible combinations of  $m$  and  $l$  that are compatible with fivefold symmetry, noting the subset of those that are also compatible with having mirror symmetry.

If the generators  $\mathbf{b}_1 \dots \mathbf{b}_l$  are *not* integrally independent modulo  $L_0$  then the modular lattice is not isomorphic to  $(\mathbb{Z}_m)^l$ . This happens when the sublattice  $L_0$  is restricted to lie along particular orientations, the first example occurring when  $L_0$  is generated by a vector of the form  $\mathbf{h} = p\mathbf{b}_1 + p\mathbf{b}_2 - p\mathbf{b}_3 - p\mathbf{b}_4$  and its images under fivefold rotations. In this case one can show that the modular lattice is isomorphic to  $\mathbb{Z}_{5p} \times \mathbb{Z}_p \times \mathbb{Z}_p \times \mathbb{Z}_p$  which, for the smallest value of  $p=2$ , requires 80 colors in each indistinguishability class. We shall not pursue these special cases any further because they do not add any additional insight into the enumeration process and because they are not relevant for our classification of color groups with up to 25 colors.

TABLE VIII. Possible indices of invariant sublattices of standard two-dimensional  $N$ -fold lattices (with mirror symmetry). The values of these indices are equal to the possible numbers of colors in an  $N$ -fold symmetric color field whose components are all indistinguishable, or equivalently, to the orders of lattice color groups  $\Gamma_e$ , compatible with an  $N$ -fold lattice. The sublattices are required to be invariant under the full point group of the  $N$ -fold lattice including its mirror reflections. The indices are calculated by evaluating the determinant in Eq. (48), restricting  $\vec{H}$  to lie either along or between mirror lines. If  $N$  is twice the power of a single prime, then two sets of indices are given, corresponding to sublattices generated by  $N$ -fold stars oriented along or between the mirror lines of  $L$ . The two sets are related by a common factor—the index of the largest sublattice generated by a star oriented between the mirror lines. If  $N$  is not twice the power of a single prime then  $L$  itself may be generated by a star oriented between the mirror lines, so there is no distinction between the two orientations.

Lattice order $N$	Point group $G$	Possible indices of sublattices, invariant under $G$
Rank 2		
4	$4mm$	$\begin{cases} h^2=1,4,9,16,25,36,49, \dots \\ 2h^2=2,8,18,32,50,72,98, \dots \end{cases}$
6	$3m,6mm$	$\begin{cases} h^2=1,4,9,16,25,36,49, \dots \\ 3h^2=3,12,27,48,75,108,147, \dots \end{cases}$
Rank 4		
8	$8mm$	$\begin{cases} (2h^2-k^2)^2=1,4,16,49,64,81,196, \dots \\ 2(2h^2-k^2)^2=2,8,32,98,128,162, \dots \end{cases}$
10	$5m,10mm$	$\begin{cases} (h^2-hk-k^2)^2=1,16,25,81,121, \dots \\ 5(h^2-hk-k^2)^2=5,80,125,405, \dots \end{cases}$
12	$12mm$	$(3h^2-k^2)^2=1,4,9,16,36,64,81,121, \dots$

The modular lattice  $L/L_0$  is left invariant under the point group  $G$  of the color field. It therefore carries an  $l$ -dimensional representation of  $G$  over  $\mathbb{Z}_m$ , i.e., every element  $g$  of  $G$  is represented by an  $l \times l$  matrix of integers modulo  $m$  given by the effect of  $g$  on the generators  $\mathbf{b}_1 \dots \mathbf{b}_l$ . The fivefold rotation  $r_5$  takes each generator  $\mathbf{b}_i$  into  $\mathbf{b}_{i+1}$  if  $i < l$ , and takes  $\mathbf{b}_l$  into the linear combination given in Eq. (49). It is therefore represented on the modular lattice by an  $l \times l$  integral matrix  $\mathcal{R}_l$  (whose coefficients may be taken modulo  $m$ ):

$$l=1: \quad \mathcal{R}_1=(h_1),$$

$$l=2: \quad \mathcal{R}_2=\begin{pmatrix} 0 & h_1 \\ 1 & h_2 \end{pmatrix},$$

$$l=3: \quad \mathcal{R}_3=\begin{pmatrix} 0 & 0 & h_1 \\ 1 & 0 & h_2 \\ 0 & 1 & h_3 \end{pmatrix},$$

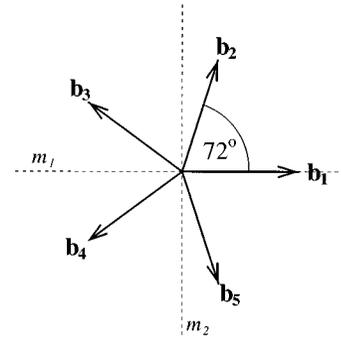


FIG. 6. Generating vectors for the two-dimensional decagonal lattice. There are five conjugate mirrors of type  $m_1$  which take vectors of the fivefold star into others in the same star, and five conjugate mirrors of type  $m_2$  which take vectors of the fivefold star into the negatives of such vectors.

$$l=4: \quad \mathcal{R}_4=\begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix}. \quad (50)$$

For the case  $l=4$  the matrix  $\mathcal{R}_4$  is given by the representation of the fivefold rotation on the full lattice  $L$ . This means that for any  $m$  there always exists a modular lattice isomorphic to  $(\mathbb{Z}_m)^4$ . This is the modular lattice one gets by taking the sublattice  $L_0$  to be the one generated by  $m\mathbf{b}_i$  ( $i=1, \dots, 4$ ). Such sublattices  $L_0$  are compatible with having mirror symmetry in the point group of the color field. If  $l < 4$  then one needs to find the integral coefficients  $h_i$  for which the matrix  $\mathcal{R}_l$  is indeed a representation of a fivefold rotation.

The sum of an arbitrary vector in the full lattice  $L$  with its four successive images under a fivefold rotation must be zero. This requirement still holds when vector arithmetic is performed modulo  $m$ . Thus, for the matrix  $\mathcal{R}_l$  to represent a fivefold rotation on  $L/L_0$ , it must satisfy

$$\mathcal{I}_l + \mathcal{R}_l + \mathcal{R}_l^2 + \mathcal{R}_l^3 + \mathcal{R}_l^4 = 0 \text{ modulo } m, \quad (51)$$

where  $\mathcal{I}_l$  is an  $l \times l$  unit matrix. Note that if condition (51) is satisfied then  $\mathcal{R}_l^5 = \mathcal{I}_l$  is satisfied as well, but the converse is not true. Condition (51) is a necessary and sufficient requirement for  $\mathcal{R}_l$  to represent a fivefold rotation on  $L/L_0$ .

Because  $L_0$  contains the negative of each of its vectors, if it is invariant under a fivefold rotation then it is also invariant under a tenfold rotation. It then follows that if it is invariant under any of the ten mirrors that leave  $L$  invariant then it is invariant under all of them. Thus to check whether for a given set of coefficients  $h_i$  the modular lattice  $L/L_0$  is compatible with having mirror symmetry in the point group it is sufficient to check for a single mirror. We choose to take the mirror that interchanges the two vectors  $\mathbf{b}_1$  and  $\mathbf{b}_{l+1}$ . If the sublattice  $L_0$  is invariant under this mirror then its representation on  $L/L_0$ , given by one of the  $l \times l$  matrices  $\mathcal{M}_l$ ,

TABLE IX. Association of rotations with indistinguishability-class permutations in the decagonal and pentagonal point groups. For each of the decagonal and pentagonal point groups  $G$ , columns 2 and 3 list all subgroups  $H$  along with the normal subgroup  $H_0$  if different from  $H$ . Column 4 lists a point group isomorphic to the quotient group  $G/H_0$ , which is isomorphic to the group of indistinguishability-class permutations induced by the cosets of  $H$  in  $G$ . Column 5 lists the number  $q$  of indistinguishability classes. Columns 6 and 7 give the actual permutations  $\delta$  and  $\mu$  associated with the generators of  $G$ —a tenfold or fivefold rotation and a mirror, respectively. Column 8 refers to the number of the star in Fig. 7 with the corresponding color point-group symmetry.

$G$	$H$	$H_0$	$G/H_0$	$q$	$\delta$	$\mu$	#
$10mm$	$10mm$	-	1	1	$\epsilon$	$\epsilon$	1
	10	-	$m$	2	$\epsilon$	$(C_1C_2)$	2
	$5m$	-	2	2	$(C_1C_2)$	$\epsilon$	3
	5	-	$2mm$	4	$(C_1C_3)(C_2C_4)$	$(C_1C_4)(C_2C_3)$	4
	$2mm$	2	$5m$	5	$(C_1C_2C_3C_4C_5)$	$(C_2C_5)(C_3C_4)$	5
	2	-	$5m$	10	$(C_1C_3 \dots C_9)(C_2C_4 \dots C_{10})$	$(C_1C_{10})(C_2C_9) \dots (C_5C_6)$	6
	$m$	1	$10mm$	10	$(C_1C_2 \dots C_{10})$	$(C_2C_{10})(C_3C_9)(C_4C_8)(C_5C_7)$	7
	1	-	$10mm$	20	$(C_1C_3 \dots C_{19})(C_2C_4 \dots C_{20})$	$(C_1C_{20})(C_2C_{19}) \dots (C_{10}C_{11})$	8
10	10	-	1	1	$\epsilon$		1
	5	-	2	2	$(C_1C_2)$		3
	2	-	5	5	$(C_1C_2C_3C_4C_5)$		5
	1	-	10	10	$(C_1C_2 \dots C_{10})$		7
$5m$	$5m$	-	1	1	$\epsilon$	$\epsilon$	9
	5	-	$m$	2	$\epsilon$	$(C_1C_2)$	10
	$m$	1	$5m$	5	$(C_1C_2C_3C_4C_5)$	$(C_2C_5)(C_3C_4)$	11
	1	-	$5m$	10	$(C_1C_3 \dots C_9)(C_2C_4 \dots C_{10})$	$(C_1C_{10})(C_2C_9) \dots (C_5C_6)$	12
5	5	-	1	1	$\epsilon$		9
	1	-	5	5	$(C_1C_2C_3C_4C_5)$		11

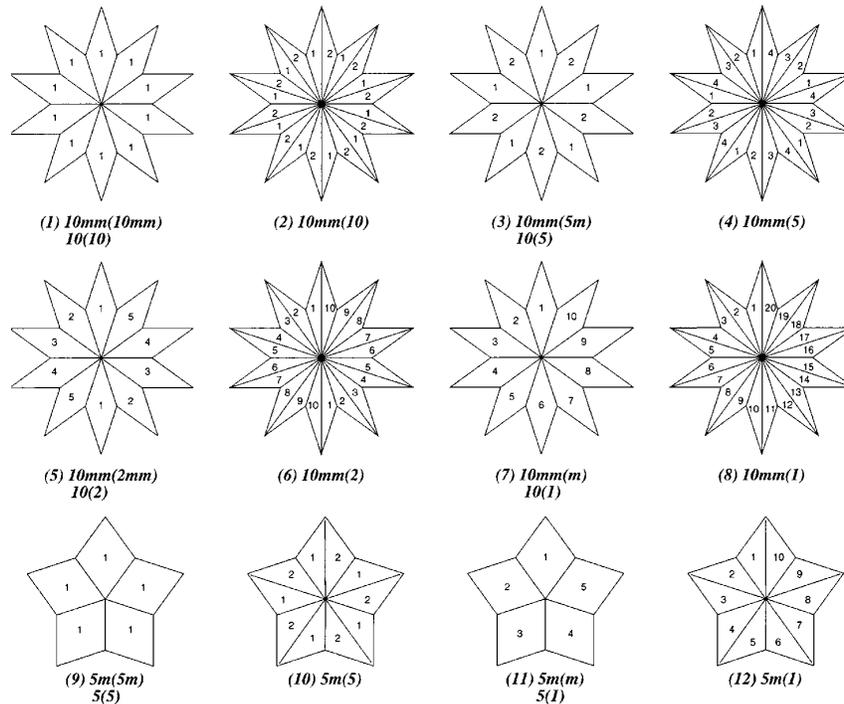


FIG. 7. Association of rotations with indistinguishability-class permutations in the decagonal and pentagonal point groups. The group-subgroup pairs  $G(H)$  are listed beneath the figures. The figures are to be used as an aid in determining the indistinguishability-class permutations associated with the different rotations of the point group as summarized in Table IX.

$$\begin{aligned}
l=1: & \mathcal{M}_1=(h_1), \\
l=2: & \mathcal{M}_2=\begin{pmatrix} h_1 & 0 \\ h_2 & 1 \end{pmatrix}, \\
l=3: & \mathcal{M}_3=\begin{pmatrix} h_1 & 0 & 0 \\ h_2 & 0 & 1 \\ h_3 & 1 & 0 \end{pmatrix}, \quad (52)
\end{aligned}$$

must satisfy the requirement that

$$\mathcal{M}_l^2 = \mathcal{I}_l \text{ modulo } m. \quad (53)$$

We use a simple MATHEMATICA program to find, for any combination of  $m$  and  $l$ , the distinct integral coefficients  $h_i$  satisfying condition (51) and for each set check whether it satisfies condition (53). Each distinct set of coefficients corresponds to a different sublattice  $L_0$  for which the modular lattice is isomorphic to  $(\mathbb{Z}_m)^l$ , or equivalently, as we show in the next section, to a distinct solution of the group compatibility conditions (21) for a lattice color group isomorphic to  $(\mathbb{Z}_m)^l$ .

### C. Values of the phase functions $\Phi_e^{\gamma}(\mathbf{k})$

Because  $\Gamma_e$  is isomorphic to  $(\mathbb{Z}_m)^l$  any element  $\gamma \in \Gamma_e$  satisfies  $\gamma^m = \epsilon$ , which through the group compatibility condition (21) requires that  $\forall \mathbf{k} \in L: m\Phi_e^{\gamma}(\mathbf{k}) \equiv 0$ , or

$$\forall \mathbf{k} \in L: \Phi_e^{\gamma}(\mathbf{k}) \equiv 0, \frac{1}{m}, \frac{2}{m} \dots \frac{m-1}{m}. \quad (54)$$

We choose a canonical set of generators  $\gamma_1 \dots \gamma_l$  for  $\Gamma_e$ , as shown in Sec. IV.C.4, for which the corresponding phase functions satisfy

$$\Phi_e^{\gamma_i}(\mathbf{b}_j) \equiv \frac{1}{m} \delta_{ij}, \quad i, j = 1 \dots l. \quad (55)$$

The values of these  $l$  generating phase functions on any other vector  $\mathbf{k} = \sum_{j=1}^l n_j \mathbf{b}_j$  in the modular lattice are given by

$$\Phi_e^{\gamma_i}(\mathbf{k}) \equiv \sum_{j=1}^l n_j \Phi_e^{\gamma_i}(\mathbf{b}_j) \equiv \frac{1}{m} \sum_{j=1}^l n_j \delta_{ij} \equiv \frac{n_i}{m}, \quad i = 1 \dots l. \quad (56)$$

Thus the values of the phase functions for the generators of  $\Gamma_e$  on the remaining generating vectors of the full lattice,  $\mathbf{b}_{l+1} \dots \mathbf{b}_4$ , are simply given by the representation of these vectors on the modular lattice in terms of the basis  $\mathbf{b}_1 \dots \mathbf{b}_l$ . These are determined by successive applications of the rotation matrix  $\mathcal{R}_l$  on the vector  $\mathbf{b}_l$ .

Tables X–XII list for  $l=1,2,3$ , the first values of  $m$  for which lattice color groups and modular lattices, isomorphic to  $(\mathbb{Z}_m)^l$ , are compatible with the tenfold lattice  $L$ . In each case, the distinct modular lattices isomorphic to  $(\mathbb{Z}_m)^l$  are listed by giving the coefficients of the vectors  $\mathbf{b}_1 \dots \mathbf{b}_5$  in terms of the basis of the modular lattice  $\mathbf{b}_1 \dots \mathbf{b}_l$ . From Eq. (56) this is equivalent to listing the values of the generating phase functions on the same

wave vectors, giving the distinct solutions to the group compatibility conditions (21). The tables also specify whether the maximal point group of color fields with such lattice color groups is  $10mm$ , containing the ten mirrors, or just 10. In the latter case the distinct modular lattices are arranged in enantiomorphic pairs in which one modular lattice is the mirror image of the other.

### D. Decagonal lattice color groups

The next step is to find the actual lattice color groups that are isomorphic to  $(\mathbb{Z}_m)^l$  and satisfy the additional requirement, of Sec. IV.C.5, that the isomorphism  $L/L_0 \cong \Gamma_e$  be invariant under the color point group. A necessary condition for this invariance to hold is that the organization of color permutations into orbits of the full permutation group  $\Gamma$  be the same as the organization of the elements of the modular lattice into orbits of the point group  $G$ . Since the lattice generators  $\mathbf{b}_1 \dots \mathbf{b}_4$  as well as  $\mathbf{b}_5$  are related by successive applications of the fivefold rotation  $r_5$ , they are in a single orbit of any decagonal or pentagonal point group. The generators  $\gamma_1 \dots \gamma_l$  of the lattice color group  $\Gamma_e$  must therefore be conjugate in  $\Gamma$ , i.e., they must have the same cycle structure. Furthermore, the permutation  $\gamma_1^{h_1} \dots \gamma_l^{h_l}$  (corresponding to the vector  $\mathbf{b}_{l+1} = \sum_{i=1}^l h_i \mathbf{b}_i$  in the isomorphism  $L/L_0 \cong \Gamma_e$ ) must also have the same cycle structure. Because, as one may directly verify, the coefficients  $h_i$  are all nonzero modulo  $m$ , this puts a serious constraint on the possible lattice color groups isomorphic to  $(\mathbb{Z}_m)^l$  that are realizable on the decagonal lattice. Each  $\gamma_i$  ( $i=1 \dots l$ ) must be a product of an equal number of  $m$ -cycles. The permutation  $\gamma_1^{h_1} \dots \gamma_l^{h_l}$  will necessarily contain a greater number of  $m$ -cycles unless the  $\gamma_i$  all permute the same colors. This leaves only a single possibility for a decagonal lattice color group, isomorphic to  $(\mathbb{Z}_m)^l$ , described as follows.

There are  $q$  indistinguishability classes with  $m^l$  colors each. One can arrange the colors in each class in an imaginary  $l$ -dimensional cube of side  $m$ , denoting each color in the  $j$ th indistinguishability class by  $l$  upper indices, each ranging from 1 to  $m$ ,  $C_j^{i_1 \dots i_l}$ . Each generator  $\gamma_1 \dots \gamma_l$  acts on a single one of the upper indices, ensuring that they all commute. This possibility satisfies the additional requirement that any product of the powers of the generators have the same structure having  $qm^{l-1}$   $m$ -cycles. We label the colors such that the first generator of  $\Gamma_e$ , for example, is given by

$$\gamma_1 = \prod_{\substack{j=1 \dots q \\ i_2=1 \dots m \\ \vdots \\ i_l=1 \dots m}} (C_j^{1, i_2, \dots, i_l} C_j^{2, i_2, \dots, i_l} \dots C_j^{m, i_2, \dots, i_l}), \quad (57)$$

with the obvious analogous forms for the rest of the generators.

Thus, for a given combination of the parameters  $m$ ,  $l$ , and  $q$ , there is only a single lattice color group  $\Gamma_e$ . The structure of the only possible lattice color groups en-

TABLE X. Two-dimensional decagonal lattice color groups isomorphic to  $Z_m$ . The distinct modular lattices isomorphic to  $Z_m$  are listed by giving the coefficients of the vectors  $\mathbf{b}_1 \dots \mathbf{b}_5$  in terms of the generator  $\mathbf{b}_1$  of the modular lattice. From Eq. (56) this is equivalent to listing the values of the generating phase function  $\Phi_e^{\gamma_1}$  on the same wave vectors, giving the distinct solutions to the group compatibility conditions (21). The right-hand column specifies whether the maximal point group of color fields with such lattice color groups is  $10mm$  or just  $10$ . In the latter case the distinct modular lattices are arranged in enantiomorphic pairs in which one modular lattice is the mirror image of the other.

$m$	$\Gamma_e \simeq Z_m (l=1)$					$G$
	$m\Phi_e^{\gamma_1}(\mathbf{b}_1)$	$m\Phi_e^{\gamma_1}(\mathbf{b}_2)$	$m\Phi_e^{\gamma_1}(\mathbf{b}_3)$	$m\Phi_e^{\gamma_1}(\mathbf{b}_4)$	$m\Phi_e^{\gamma_1}(\mathbf{b}_5)$	
5	1	1	1	1	1	$10mm$
11	1	3	9	5	4	10
	1	4	5	9	3	10
	1	5	3	4	9	10
	1	9	4	3	5	10
31	1	2	4	8	16	10
	1	16	8	4	2	10
	1	4	16	2	8	10
	1	8	2	16	4	10
41	1	10	18	16	37	10
	1	37	16	18	10	10
	1	16	10	37	18	10
	1	18	37	10	16	10
55	1	16	36	26	31	10
	1	31	26	36	16	10
	1	26	16	31	36	10
	1	36	31	16	26	10
61	1	9	20	58	34	10
	1	34	58	20	9	10
	1	20	34	9	58	10
	1	58	9	34	20	10
71	1	5	25	54	57	10
	1	57	54	25	5	10
	1	25	57	5	54	10
	1	54	5	57	25	10

tures that all decagonal and pentagonal color space groups are simple, as defined in Sec. IV.B.2. This situation is analogous to the example given in Sec. IV.C.6 in the case of the triangular lattice.

**E. Decagonal and pentagonal color point groups**

We are now at a position where we have all the required information to construct the decagonal and pentagonal color point groups. Given the number  $n$  of colors in the color field we first consider all possible factorizations of  $n$  into  $q$  indistinguishability classes, each containing  $m^l$  colors. The possible values of  $q$  are taken from Table IX. If  $l=1, 2,$  or  $3$  then the possible

values of  $m$  are taken from the corresponding Tables X–XII. If  $l=4$  then  $m$  can take any integer value. For each combination of the parameters  $q, m,$  and  $l$  we consider all the combinations of  $G$  and  $H$  from Table IX for which  $q$  is the index of  $H$  in  $G$ , excluding cases in which  $G$  contains any mirrors if the values of  $m$  and  $l$  are incompatible with mirror symmetry.

The generators of the color point group are  $(e, \gamma_1), \dots, (e, \gamma_l), (r, \delta)$ , and possibly also  $(m, \mu)$ , where  $r$  is either a tenfold rotation  $r_{10}$  (if  $G$  is  $10mm$  or  $10$ ) or a fivefold rotation  $r_5$  (if  $G$  is  $5m1, 51m,$  or  $5$ ), and  $m$  is either a mirror of type  $m_1$  (if  $G$  is  $10mm$  or  $5m1$ ) or type  $m_2$  (if  $G$  is  $51m$ ), as defined in Fig. 6. The color permutations  $\gamma_i$ , generating the lattice color group  $\Gamma_e$ , are given by Eq. (57) for each possible lattice color

TABLE XI. Two-dimensional decagonal lattice color groups isomorphic to  $Z_m \times Z_m$ . The distinct modular lattices isomorphic to  $Z_m \times Z_m$  are listed by giving the coefficients of the vectors  $\mathbf{b}_1 \dots \mathbf{b}_5$  in terms of the basis  $\mathbf{b}_1, \mathbf{b}_2$  of the modular lattice. From Eq. (56) this is equivalent to listing the values of the generating phase functions on the same wave vectors, giving the distinct solutions to the group compatibility conditions (21). The right-hand column specifies whether the maximal point group of color fields with such lattice color groups is  $10mm$  or just  $10$ . In the latter case the distinct modular lattices are arranged in enantiomorphic pairs in which one modular lattice is the mirror image of the other.

$m$	$\Gamma_e \simeq Z_m \times Z_m$ ( $l=2$ )					$G$
	$m\Phi_e^{\gamma_i}(\mathbf{b}_1)$	$m\Phi_e^{\gamma_i}(\mathbf{b}_2)$	$m\Phi_e^{\gamma_i}(\mathbf{b}_3)$	$m\Phi_e^{\gamma_i}(\mathbf{b}_4)$	$m\Phi_e^{\gamma_i}(\mathbf{b}_5)$	
5	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 4 \\ 2 \end{pmatrix}$	$\begin{pmatrix} 3 \\ 3 \end{pmatrix}$	$\begin{pmatrix} 2 \\ 4 \end{pmatrix}$	$10mm$
11	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 3 \end{pmatrix}$	$\begin{pmatrix} 8 \\ 8 \end{pmatrix}$	$\begin{pmatrix} 3 \\ 10 \end{pmatrix}$	$10mm$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 7 \end{pmatrix}$	$\begin{pmatrix} 4 \\ 4 \end{pmatrix}$	$\begin{pmatrix} 7 \\ 10 \end{pmatrix}$	$10mm$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 2 \\ 9 \end{pmatrix}$	$\begin{pmatrix} 7 \\ 6 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 6 \end{pmatrix}$	$10$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 6 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 6 \\ 7 \end{pmatrix}$	$\begin{pmatrix} 9 \\ 2 \end{pmatrix}$	$10$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 7 \\ 8 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 5 \end{pmatrix}$	$\begin{pmatrix} 2 \\ 8 \end{pmatrix}$	$10$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 8 \\ 2 \end{pmatrix}$	$\begin{pmatrix} 5 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 8 \\ 7 \end{pmatrix}$	$10$
19	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 18 \\ 4 \end{pmatrix}$	$\begin{pmatrix} 15 \\ 15 \end{pmatrix}$	$\begin{pmatrix} 4 \\ 18 \end{pmatrix}$	$10mm$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 18 \\ 14 \end{pmatrix}$	$\begin{pmatrix} 5 \\ 5 \end{pmatrix}$	$\begin{pmatrix} 14 \\ 18 \end{pmatrix}$	$10mm$
29	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 28 \\ 5 \end{pmatrix}$	$\begin{pmatrix} 24 \\ 24 \end{pmatrix}$	$\begin{pmatrix} 5 \\ 28 \end{pmatrix}$	$10mm$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 28 \\ 23 \end{pmatrix}$	$\begin{pmatrix} 6 \\ 6 \end{pmatrix}$	$\begin{pmatrix} 23 \\ 28 \end{pmatrix}$	$10mm$
31	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 30 \\ 12 \end{pmatrix}$	$\begin{pmatrix} 19 \\ 19 \end{pmatrix}$	$\begin{pmatrix} 12 \\ 30 \end{pmatrix}$	$10mm$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 30 \\ 18 \end{pmatrix}$	$\begin{pmatrix} 13 \\ 13 \end{pmatrix}$	$\begin{pmatrix} 18 \\ 30 \end{pmatrix}$	$10mm$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 15 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 26 \\ 22 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 29 \end{pmatrix}$	$10$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 29 \\ 20 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 26 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 15 \end{pmatrix}$	$10$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 23 \\ 6 \end{pmatrix}$	$\begin{pmatrix} 14 \\ 28 \end{pmatrix}$	$\begin{pmatrix} 24 \\ 27 \end{pmatrix}$	$10$
	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 27 \\ 24 \end{pmatrix}$	$\begin{pmatrix} 28 \\ 14 \end{pmatrix}$	$\begin{pmatrix} 6 \\ 23 \end{pmatrix}$	$10$

group listed in Tables X–XII. The coset  $\delta\Gamma_e$ , containing all the color permutations that are paired in the color point group with  $r$ , is uniquely determined. Each of its elements must permute the indistinguishability classes

according to the permutation of the left cosets of  $H$  in  $G$ , which is induced by  $r$ , and then permute the colors within the classes so as to induce the automorphism of  $\Gamma_e$ , required by the invariance of the isomorphism

TABLE XII. Two-dimensional decagonal lattice color groups isomorphic to  $Z_m \times Z_m \times Z_m$ . The distinct modular lattices isomorphic to  $Z_m \times Z_m \times Z_m$  are listed by giving the coefficients of the vectors  $\mathbf{b}_1 \dots \mathbf{b}_5$  in terms of the basis  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  of the modular lattice. From Eq. (56) this is equivalent to listing the values of the generating phase functions on the same wave vectors, giving the distinct solutions to the group compatibility conditions (21). The right-hand column specifies whether the maximal point group of color fields with such lattice color groups is  $10mm$  or just  $10$ . In the latter case the distinct modular lattices are arranged in enantiomorphic pairs in which one modular lattice is the mirror image of the other.

$m$	$\Gamma_e \simeq Z_m \times Z_m \times Z_m \ (l=3)$					$G$
	$m\Phi_e^{\gamma_i}(\mathbf{b}_1)$	$m\Phi_e^{\gamma_i}(\mathbf{b}_2)$	$m\Phi_e^{\gamma_i}(\mathbf{b}_3)$	$m\Phi_e^{\gamma_i}(\mathbf{b}_4)$	$m\Phi_e^{\gamma_i}(\mathbf{b}_5)$	
5	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$	$\begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix}$	$10mm$
11	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 3 \\ 1 \\ 6 \end{pmatrix}$	$\begin{pmatrix} 7 \\ 9 \\ 4 \end{pmatrix}$	10
	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 4 \\ 9 \\ 7 \end{pmatrix}$	$\begin{pmatrix} 6 \\ 1 \\ 3 \end{pmatrix}$	10
	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 5 \\ 8 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 5 \\ 2 \\ 9 \end{pmatrix}$	10
	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 9 \\ 2 \\ 5 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 8 \\ 5 \end{pmatrix}$	10
31	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 2 \\ 6 \\ 14 \end{pmatrix}$	$\begin{pmatrix} 28 \\ 24 \\ 16 \end{pmatrix}$	10
	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 16 \\ 24 \\ 28 \end{pmatrix}$	$\begin{pmatrix} 14 \\ 6 \\ 2 \end{pmatrix}$	10
	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 4 \\ 20 \\ 22 \end{pmatrix}$	$\begin{pmatrix} 26 \\ 10 \\ 8 \end{pmatrix}$	10
	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 8 \\ 10 \\ 26 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 20 \\ 4 \end{pmatrix}$	10

$\Gamma_e \simeq L/L_0$  under  $(r, \delta)$ . The coset of  $\Gamma_e$  containing  $\mu$  is determined in a similar way. The freedom to choose the actual coset representatives  $\delta$  and  $\mu$  will be utilized in the next section. This completely specifies all the possible color point groups, except for the special cases when the lattice color group is *not* isomorphic to  $(Z_m)^l$ . We explicitly list, in Table XIII, all decagonal and pentagonal color point groups for color fields with up to 25 colors. Each color point group is given a sequential number but may also be uniquely specified by the symbol  $(G, H, H_0, G_\epsilon | \Gamma_e)$ . In this notation, the color point groups of the tilings of Figs. 3 and 4 are  $(10mm, 10mm, 10mm, 5m1 | Z_5)$  and  $(10mm, 2mm, 2, 2 | Z_1)$ , respectively.

**F. Decagonal and pentagonal color space-group types**

In order to complete the enumeration of all color space-group types we need to find for every color point

group the distinct sets of phase functions that satisfy the group compatibility conditions (11). As always, we specify each given set by listing the values of the phase functions corresponding to the generators of the color point group on the generating vectors of the lattice  $\mathbf{b}_1 \dots \mathbf{b}_4$ .

The values of the gauge-invariant phase functions  $\Phi_e^{\gamma_i}$  ( $i=1 \dots l$ ) on the lattice-generating vectors are already given in Tables X–XII for  $l=1, 2$ , or  $3$ , and by Eq. (55) for  $l=4$ . We need only specify the phase function  $\Phi_r^\delta$  and possibly also  $\Phi_m^\mu$ . We show below that both these phase functions can be taken to be zero everywhere on the lattice.

We choose to consider enantiomorphic pairs of gauge-equivalence classes of phase functions as distinct space-group types. Thus the entries of Tables X–XII along with Eq. (55) for the case  $l=4$  give not only the gauge-

TABLE XIII. Two-dimensional decagonal and pentagonal color point groups for color fields with up to 25 colors. Color point groups are arranged according to the number  $n$  of colors. In each case the groups are listed in separate sections corresponding to the decomposition of  $n$  into a product of the number  $q$  of indistinguishability classes and the number  $m^l$  of colors in each class. The left-hand side of the table lists the point groups  $G$ ,  $H$ ,  $H_0$ , and  $G_\epsilon$  along with two point groups isomorphic to the quotient groups  $G/H_0$  and  $G/G_\epsilon$ . A point group is not listed if it is equal to the one on its left. The right-hand side of the table explicitly lists the color point groups by giving their generators. These are the generators  $(e, \gamma_i)$ , expressed generally in Eq. (57), along with  $(r, \delta)$  and possibly also  $(m, \mu)$ . Since all decagonal and pentagonal color point groups are simple, the color permutations are all given as a product of a barred permutation, which permutes whole indistinguishability classes of colors (operating on the lower indices of the colors  $C_j^k$ ), and an unbarred permutation, which simultaneously permutes colors within each class (operating on the upper indices of the colors  $C_j^k$ ). In most cases the permutations  $\delta$  and  $\mu$  are given explicitly; in some cases, to save space, they are given only in terms of their effect on the generators  $\gamma_i$  of the lattice color group. In the cases with  $\Gamma_e \simeq \mathbb{Z}_{11}$  the integer  $h_1$  refers to the value of  $11\Phi_e^*(\mathbf{b}_2)$  given in Table X. As notation for the color point groups we use either (1) the sequential number listed in the leftmost column (the additional number in parentheses refers to the numbering of color space-group types), or (2) the symbol  $(G, H, H_0, G_\epsilon | \Gamma_e)$ . For example, the color point group (or color space-group type) number 10.b.1 is denoted by  $(10mm, 10, 10, 5 | \mathbb{Z}_5)$ .

2 colors							
No.	$G$	$\Gamma_e \simeq \mathbb{Z}_1, q=2$			$G/H_0$	$G/G_\epsilon$	$\bar{\delta} = \bar{\mu} = (C_1 C_2)$ Generators of the color point group
		$H$	$H_0$	$G_\epsilon$			
2.1	10mm	10	-	-	$m$	$m$	$(r_{10}, \epsilon), (m_1, \bar{\mu})$
2.2	10mm	51m	-	-	2	2	$(r_{10}, \bar{\delta}), (m_1, \bar{\mu})$
2.3	10mm	5m1	-	-	2	2	$(r_{10}, \bar{\delta}), (m_1, \epsilon)$
2.4	10	5	-	-	2	2	$(r_{10}, \bar{\delta})$
2.5	5m1	5	-	-	$m$	$m$	$(r_5, \epsilon), (m_1, \bar{\mu})$
2.6	51m	5	-	-	$m$	$m$	$(r_5, \epsilon), (m_2, \bar{\mu})$

4 colors							
No.	$G$	$\Gamma_e \simeq \mathbb{Z}_1, q=4$			$G/H_0$	$G/G_\epsilon$	$\bar{\delta} = (C_1 C_3)(C_2 C_4), \bar{\mu} = (C_1 C_4)(C_2 C_3)$ Generators of the color point group
		$H$	$H_0$	$G_\epsilon$			
4.1	10mm	5	-	-	2mm	2mm	$(r_{10}, \bar{\delta}), (m_1, \bar{\mu})$

5 colors							
No.	$G$	$\Gamma_e \simeq \mathbb{Z}_1, q=5$			$G/H_0$	$G/G_\epsilon$	$\bar{\delta} = (C_1 C_2 C_3 C_4 C_5), \bar{\mu} = (C_2 C_5)(C_3 C_4)$ Generators of the color point group
		$H$	$H_0$	$G_\epsilon$			
5.a.1	10mm	2mm	2	-	5m	5m	$(r_{10}, \bar{\delta}), (m_1, \bar{\mu})$
5.a.2	10	2	2	-	5	5	$(r_{10}, \bar{\delta})$
5.a.3	5m1	1m1	1	-	5m	5m	$(r_5, \bar{\delta}), (m_1, \bar{\mu})$
5.a.4	51m	11m	1	-	5m	5m	$(r_5, \bar{\delta}), (m_2, \bar{\mu})$
5.a.5	5	1	1	-	5	5	$(r_5, \bar{\delta})$

$\Gamma_e \simeq \mathbb{Z}_5, q=1$							
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	$\gamma = (C^1 C^2 C^3 C^4 C^5), \delta = \mu = (C^2 C^5)(C^3 C^4)$ Generators of the color point group
5.b.2	10	10	-	5	1	2	$(e, \gamma), (r_{10}, \delta)$
5.b.3	5m1	5m1	-	5m1	1	1	$(e, \gamma), (r_5, \epsilon), (m_1, \epsilon)$
5.b.4	51m	51m	-	5	1	$m$	$(e, \gamma), (r_5, \epsilon), (m_2, \mu)$
5.b.5	5	5	-	5	1	1	$(e, \gamma), (r_5, \epsilon)$

TABLE XIII. (Continued).

							10 colors		
							$\Gamma_e \approx Z_1, q=10$		
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	Generators of the color point group		
10.a.1	10mm	2	2	-	5m	5m	$\bar{\delta}_1 = (C_1 C_3 \dots C_9)(C_2 C_4 \dots C_{10}), \bar{\delta}_2 = (C_1 C_2 \dots C_{10})$ $\bar{\mu}_1 = (C_1 C_{10}) \dots (C_5 C_6), \bar{\mu}_2 = (C_2 C_{10})(C_3 C_9)(C_4 C_8)(C_5 C_7)$		
10.a.2	10mm	11m	1	-	10mm	10mm	$(r_{10}, \bar{\delta}_1), (m_1, \bar{\mu}_1)$		
10.a.3	10mm	1m1	1	-	10mm	10mm	$(r_{10}, \bar{\delta}_2), (m_1, \bar{\mu}_1)$		
10.a.4	10	1	-	-	10	10	$(r_{10}, \bar{\delta}_2), (m_1, \bar{\mu}_2)$		
10.a.5	5m1	1	-	-	5m	5m	$(r_{10}, \bar{\delta}_2)$		
10.a.6	51m	1	-	-	5m	5m	$(r_5, \bar{\delta}_1), (m_1, \bar{\mu}_1)$ $(r_5, \bar{\delta}_1), (m_2, \bar{\mu}_1)$		
							$\Gamma_e \approx Z_5, q=2$		
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	Generators of the color point group		
10.b.1	10mm	10	-	5	m	2mm	$\gamma = \prod_{j=1,2} (C_j^1 C_j^2 C_j^3 C_j^4 C_j^5), \delta = \mu = \prod_{j=1,2} (C_j^2 C_j^5)(C_j^3 C_j^4)$ $\bar{\delta} = \bar{\mu} = \prod_{i=1, \dots, 5} (C_i^1 C_i^2)$		
10.b.2	10mm	51m	-	5	2	2	$(e, \gamma), (r_{10}, \delta), (m_1, \bar{\mu})$		
10.b.3	10mm	5m1	-	5	2	2	$(e, \gamma), (r_{10}, \delta \bar{\delta}), (m_1, \bar{\mu})$		
10.b.4	10	5	-	-	2	2	$(e, \gamma), (r_{10}, \delta \bar{\delta}), (m_1, \epsilon)$		
10.b.5	5m1	5	-	-	m	m	$(e, \gamma), (r_{10}, \delta \bar{\delta})$		
10.b.6	51m	5	-	-	m	m	$(e, \gamma), (r_5, \epsilon), (m_1, \bar{\mu})$ $(e, \gamma), (r_5, \epsilon), (m_2, \mu \bar{\mu})$		
							11 colors		
							$\Gamma_e \approx Z_{11}, q=1$		
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	Generators of the color point group		
11.1(1-4)	10	10	-	1	1	10	$\gamma = (C^1 C^2 \dots C^{11}), \delta_{10}: \gamma \rightarrow \gamma^{-h_1^3}, \delta_5 = \delta_{10}^2: \gamma \rightarrow \gamma^{h_1}$		
11.2(1-4)	5	5	-	1	1	5	$(e, \gamma), (10, \delta_{10})$ $(e, \gamma), (5, \delta_5)$		
							16 colors		
							$\Gamma_e \approx (Z_2)^4, q=1$		
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	Generators of the color point group		
16.1	10mm	10mm	-	2	1	5m	$\gamma_1 = \prod_{i_2, i_3, i_4=1,2} (C^{1, i_2, i_3, i_4} C^{2, i_2, i_3, i_4})$ $\gamma_2 = \prod_{i_1, i_3, i_4=1,2} (C^{i_1, 1, i_3, i_4} C^{i_1, 2, i_3, i_4})$ $\gamma_3 = \prod_{i_1, i_2, i_4=1,2} (C^{i_1, i_2, 1, i_4} C^{i_1, i_2, 2, i_4})$ $\gamma_4 = \prod_{i_1, i_2, i_3=1,2} (C^{i_1, i_2, i_3, 1} C^{i_1, i_2, i_3, 2})$ $\bar{\delta}_5: \gamma_1 \rightarrow \gamma_2 \rightarrow \gamma_3 \rightarrow \gamma_4 \rightarrow \gamma_1 \gamma_2 \gamma_3 \gamma_4 \rightarrow \gamma_1, \delta_{10} = \bar{\delta}_5^3$ $\mu: \gamma_1 \rightarrow \gamma_4 \rightarrow \gamma_1; \gamma_2 \rightarrow \gamma_3 \rightarrow \gamma_2$		
16.2	10	10	-	2	1	5	$(e, \gamma_1), (e, \gamma_2), (e, \gamma_3), (e, \gamma_4), (r_{10}, \delta_{10}), (m_1, \mu)$		
16.3	5m1	5m1	-	1	1	5m	$(e, \gamma_1), (e, \gamma_2), (e, \gamma_3), (e, \gamma_4), (r_{10}, \delta_{10})$		
16.4	51m	51m	-	1	1	5m	$(e, \gamma_1), (e, \gamma_2), (e, \gamma_3), (e, \gamma_4), (r_5, \delta_5), (m_1, \mu)$		
16.5	5	5	-	1	1	5	$(e, \gamma_1), (e, \gamma_2), (e, \gamma_3), (e, \gamma_4), (r_5, \delta_5), (m_2, \mu)$ $(e, \gamma_1), (e, \gamma_2), (e, \gamma_3), (e, \gamma_4), (r_5, \delta_5)$		

TABLE XIII. (Continued).

							20 colors
							$\bar{\delta} = (C_1 C_3 \dots C_{19})(C_2 C_4 \dots C_{20}), \bar{\mu} = (C_1 C_{20}) \dots (C_{10} C_{11})$
							Generators of the color point group
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	
$\Gamma_e \simeq Z_1, q=20$							
20.a.1	10mm	1	-	-	10mm	10mm	$(r_{10}, \bar{\delta}), (m_1, \bar{\mu})$
$\Gamma_e \simeq Z_5, q=4$							
							$\gamma = \prod_{j=1, \dots, 4} (C_j^1 C_j^2 C_j^3 C_j^4 C_j^5), \delta = \prod_{j=1, \dots, 4} (C_j^2 C_j^5)(C_j^3 C_j^4)$
							$\bar{\delta} = \prod_{i=1, \dots, 5} (C_1^i C_3^i)(C_2^i C_4^i), \bar{\mu} = \prod_{i=1, \dots, 5} (C_1^i C_4^i)(C_2^i C_3^i)$
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	Generators of the color point group
20.b.1	10mm	5	-	-	2mm	2mm	$(e, \gamma), (r_{10}, \delta \bar{\delta}), (m_1, \bar{\mu})$
							22 colors
$\Gamma_e \simeq Z_{11}, q=2$							
							$\gamma = \prod_{j=1, 2} (C_j^1 C_j^2 \dots C_j^{11}), \delta: \gamma \rightarrow \gamma^{-h_1^3}$
							$\bar{\delta} = \prod_{i=1, \dots, 11} (C_1^i C_2^i)$
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	Generators of the color point group
22.1(1-4)	10	5	-	1	2	10	$(e, \gamma), (10, \delta \bar{\delta})$
							25 colors
$\Gamma_e \simeq Z_5, q=5$							
							$\gamma = \prod_{j=1, \dots, 5} (C_j^1 C_j^2 C_j^3 C_j^4 C_j^5), \delta = \mu = \prod_{j=1, \dots, 5} (C_j^2 C_j^5)(C_j^3 C_j^4)$
							$\bar{\delta} = \prod_{i=1, \dots, 5} (C_1^i C_2^i C_3^i C_4^i C_5^i), \bar{\mu} = \prod_{i=1, \dots, 5} (C_2^i C_5^i)(C_3^i C_4^i)$
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	Generators of the color point group
25.a.1	10mm	2mm	2	1	5m	10mm	$(e, \gamma), (r_{10}, \delta \bar{\delta}), (m_1, \bar{\mu})$
25.a.2	10	2	2	1	5	10	$(e, \gamma), (r_{10}, \delta \bar{\delta})$
25.a.3	5m1	1m1	1	-	5m	5m	$(e, \gamma), (r_5, \bar{\delta}), (m_1, \bar{\mu})$
25.a.4	51m	11m	1	-	5m	5m	$(e, \gamma), (r_5, \bar{\delta}), (m_2, \mu \bar{\mu})$
25.a.5	5	1	1	-	5	5	$(e, \gamma), (r_5, \bar{\delta})$
$\Gamma_e \simeq (Z_5)^2, q=1$							
							$\gamma_1 = \prod_{i_2=1, \dots, 5} (C^{1, i_2} C^{2, i_2} \dots C^{5, i_2}), \gamma_2 = \prod_{i_1=1, \dots, 5} (C^{i_1, 1} C^{i_1, 2} \dots C^{i_1, 5})$
							$\delta_{10}: \gamma_1 \rightarrow \gamma_1^2 \gamma_2^2 \rightarrow \gamma_2 \rightarrow \gamma_1^3 \gamma_2, \delta_5 = \delta_{10}^2: \gamma_1 \rightarrow \gamma_2 \rightarrow \gamma_1^4 \gamma_2^2$
							$\mu_1: \gamma_1 \rightarrow \gamma_2 \rightarrow \gamma_1, \mu_2: \gamma_1 \rightarrow \gamma_2^4; \gamma_2 \rightarrow \gamma_1^4$
No.	$G$	$H$	$H_0$	$G_\epsilon$	$G/H_0$	$G/G_\epsilon$	Generators of the color point group
25.b.1	10mm	10mm	-	1	1	10mm	$(e, \gamma_1), (e, \gamma_2), (r_{10}, \delta_{10}), (m_1, \mu_1)$
25.b.2	10	10	-	1	1	10	$(e, \gamma_1), (e, \gamma_2), (r_{10}, \delta_{10})$
25.b.3	5m1	5m1	-	1	1	5m	$(e, \gamma_1), (e, \gamma_2), (r_5, \delta_5), (m_1, \mu_1)$
25.b.4	51m	51m	-	1	1	5m	$(e, \gamma_1), (e, \gamma_2), (r_5, \delta_5), (m_2, \mu_2)$
25.b.5	5	5	-	1	1	5	$(e, \gamma_1), (e, \gamma_2), (r_5, \delta_5)$

equivalence classes but also the scale-equivalence classes and therefore the color space-group types themselves. Combined with Table XIII they provide an explicit listing of all decagonal and pentagonal color space-group types for color fields with up to 25 colors.

1. Making  $\Phi_r^\delta$  vanish everywhere on the lattice

We can make the phases  $\Phi_r^\delta(\mathbf{b}_i) \equiv 0$  ( $i=1 \dots 4$ ) and therefore the phase function  $\Phi_r^\delta$  zero everywhere on the lattice with a gauge transformation (17) given by the gauge function<sup>14</sup>

$$\chi(\mathbf{b}_i) = \frac{1}{n} \Phi_r^\delta((1-r^{n-1}) \dots (1-r^2)\mathbf{b}_i), \quad i=1 \dots 4, \tag{58}$$

where  $n=10$  or  $5$  depending on whether  $r$  is the tenfold rotation  $r_{10}$  or the fivefold rotation  $r_5$ , and where an operator  $(1-g)$  applied to a vector  $\mathbf{k}$  is simply  $\mathbf{k}-g\mathbf{k}$ . Using the identity<sup>15</sup>

$$n = (1-r^{n-1})(1-r^{n-2}) \dots (1-r) \tag{59}$$

we establish that the gauge transformation determined by Eq. (58) changes  $\Phi_r^\delta(\mathbf{b}_i)$  by

$$\Delta\Phi_r^\delta(\mathbf{b}_i) \equiv \chi(r\mathbf{b}_i - \mathbf{b}_i) \equiv -\chi((1-r)\mathbf{b}_i) \equiv -\Phi_r^\delta(\mathbf{b}_i), \tag{60}$$

$i=1 \dots 4,$

thereby setting the phase function  $\Phi_r^\delta$  to zero everywhere on the lattice.

2. Choosing  $\delta$  and  $\mu$  to make  $\Phi_m^\mu$  vanish everywhere on the lattice

If a mirror  $m$  is among the generators of the point group  $G$  then one may verify that within the coset of  $\Gamma_e$ , paired with  $m$  in the color point group, there always exists at least one color permutation  $\mu$  satisfying  $\mu^2 = \epsilon$ . We pick  $(m, \mu)$  as a generator for the color point group. We may similarly pick the other generator  $(r, \delta)$  such that the color permutation  $\delta_5\mu$ , paired with the mirror  $r_5m$ , also satisfies  $(\delta_5\mu)^2 = \epsilon$  (here  $\delta_5 = \delta$ , or  $\delta^2$  depending on whether  $r=r_5$ , or  $r_{10}$ ). With this choice of color permutations for the generators of the color point group the following relations hold among the generators:

$$(m, \mu)^2 = (e, \epsilon) \tag{61}$$

and

$$(r_5, \delta_5)(m, \mu)(r_5, \delta_5) = (m, \mu). \tag{62}$$

Since we are in a gauge with  $\Phi_{r_5}^{\delta_5}(\mathbf{b}_i) \equiv 0$ , the generating relation (62) gives via successive applications of the group compatibility condition (11) the condition that

$\Phi_m^\mu(\mathbf{b}_i) \equiv \Phi_m^\mu(\mathbf{b}_1)$ ,  $i=2 \dots 5$ . Because the sum of the five vectors  $\mathbf{b}_1 \dots \mathbf{b}_5$  is zero, linearity of the phase function requires that

$$5\Phi_m^\mu(\mathbf{b}_1) \equiv 0. \tag{63}$$

If the point group  $G$  is  $10mm$  or  $5m1$ , then  $m$  is of type  $m_1$ , leaving the vector  $\mathbf{b}_1$  invariant, and one gets through the generating relation (61) the additional requirement that

$$2\Phi_m^\mu(\mathbf{b}_1) \equiv 0. \tag{64}$$

The two requirements, given by Eqs. (63) and (64), are satisfied only if  $\Phi_m^\mu(\mathbf{b}_i) \equiv 0$  for  $i=1 \dots 5$ , establishing that  $\Phi_m^\mu$  vanishes everywhere on the lattice.

If the point group  $G$  is  $51m$  then  $m$  is of type  $m_2$ , taking the vector  $\mathbf{b}_1$  to  $-\mathbf{b}_1$ , and one has only the requirement of Eq. (63) that  $\Phi_m^\mu(\mathbf{b}_i) \equiv j/5$  for some integer  $j$  between 0 and 4. In this case, consider the additional gauge function  $\chi^-(\mathbf{b}_i) \equiv 1/5$ . The gauge transformation determined by such a gauge function changes  $\Phi_m^\mu(\mathbf{b}_1)$  by

$$\Delta\Phi_m^\mu(\mathbf{b}_1) \equiv \chi^-(m\mathbf{b}_1 - \mathbf{b}_1) \equiv \chi^-(-2\mathbf{b}_1) \equiv -2/5. \tag{65}$$

Since 2 and 5 are both prime, repeated applications of the gauge transformation (65) can change the phases  $\Phi_m^\mu(\mathbf{b}_i)$  by an arbitrary multiple of  $1/5$  setting  $\Phi_m^\mu$  to zero everywhere on the lattice. Note that the gauge transformation (65) does not alter the value of  $\Phi_r^\delta(\mathbf{b}_i) \equiv 0$ ,  $r$  being  $r_5$  in this case, because

$$\Delta\phi_r^\delta(\mathbf{b}_i) \equiv \chi^-(\mathbf{b}_{i+1} - \mathbf{b}_i) \equiv 0, \quad i=1 \dots 4. \tag{66}$$

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<sup>14</sup>This is the same gauge function used in the uncolored case by Rabson *et al.* (1991, p. 708).

<sup>15</sup>One may use the relation  $r^n = e=1$  to verify directly that this identity holds for the special cases  $n=5, 10$  or see the general proof given by Rabson *et al.* (1991, p. 708).

## APPENDIX: INDISTINGUISHABILITY OF QUASIPERIODIC MULTICOMPONENT FIELDS

### 1. Quasiperiodic multicomponent fields

Let us consider the more general case of a multicomponent quasiperiodic field  $\vec{\psi}(\mathbf{r})$  whose components  $\psi_\alpha(\mathbf{r})$  could specify a tensor field, as in magnetically ordered solids or liquid crystals, or a number of fields unrelated to spatial orientation, such as the components in a Potts model or—the case on which we focus in this paper—the fields of different colors in a quasiperiodic colored crystal. By “quasiperiodic” we mean that the Fourier expansion of the multicomponent field

$$\vec{\psi}(\mathbf{r}) = \sum_{\mathbf{k} \in L} \vec{\psi}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} \quad (\text{A1})$$

is well defined and requires at most a countable infinity of plane waves. The lattice  $L$  consists of all integral linear combinations of wave vectors  $\mathbf{k}$  at which at least one component of the field has a nonvanishing Fourier coefficient  $\psi_\alpha(\mathbf{k})$ .

### 2. The theorem

We define two quasiperiodic multicomponent fields  $\vec{\psi}(\mathbf{r})$  and  $\vec{\psi}'(\mathbf{r})$  to be *indistinguishable* if the positionally

averaged autocorrelation functions of  $\vec{\psi}(\mathbf{r})$  of any order and for any choice of components are identical to the corresponding autocorrelation functions of  $\vec{\psi}'(\mathbf{r})$ . This definition implies, as in the scalar case, that the two multicomponent fields have the same spatial distribution of bounded substructures on any scale.

We prove below that an equivalent statement of indistinguishability is that the Fourier coefficients of the two fields are related by

$$\vec{\psi}(\mathbf{k}) = e^{2\pi i \chi(\mathbf{k})} \vec{\psi}'(\mathbf{k}), \quad (\text{A2})$$

where  $\chi$ , called a *gauge function*, is linear modulo an integer over the lattice  $L$  of wave vectors. This is similar to the statement of indistinguishability of two single component densities with the added requirement that it be the same gauge function  $\chi$  which relates *all* the components of the two fields.

### 3. The proof

The equality of all autocorrelation functions is the statement that

$$\begin{aligned} \lim_{V \rightarrow \infty} \frac{1}{V} \int d\mathbf{r} \psi_{\alpha_1}(\mathbf{r}_1 - \mathbf{r}) \cdots \psi_{\alpha_j}(\mathbf{r}_j - \mathbf{r}) \cdot \psi_{\alpha_{j+1}}^*(\mathbf{r}_{j+1} - \mathbf{r}) \cdots \psi_{\alpha_n}^*(\mathbf{r}_n - \mathbf{r}) \\ = \lim_{V \rightarrow \infty} \frac{1}{V} \int d\mathbf{r} \psi'_{\alpha_1}(\mathbf{r}_1 - \mathbf{r}) \cdots \psi'_{\alpha_j}(\mathbf{r}_j - \mathbf{r}) \cdot \psi'_{\alpha_{j+1}}^*(\mathbf{r}_{j+1} - \mathbf{r}) \cdots \psi'_{\alpha_n}^*(\mathbf{r}_n - \mathbf{r}) \end{aligned} \quad (\text{A3})$$

for any choice of the components  $\alpha_1 \dots \alpha_n$  and of the indices  $j$  and  $n$ . The asterisk denotes complex conjugation, should the multicomponent field be complex.

The Fourier decomposition of the individual components of  $\vec{\psi}(\mathbf{r})$  is given by

$$\begin{aligned} \psi_\alpha(\mathbf{r}) &= \sum_{\mathbf{k} \in L_\alpha} \psi_\alpha(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}}, \\ \psi_\alpha^*(\mathbf{r}) &= \sum_{\mathbf{k} \in L_\alpha} \psi_\alpha^*(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{r}} = \sum_{\mathbf{k} \in L_\alpha} \psi_\alpha^*(-\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}}, \end{aligned} \quad (\text{A4})$$

where the lattice  $L_\alpha$  is the set of all integral linear combinations of wave vectors with nonvanishing  $\psi_\alpha(\mathbf{k})$ , which in general may differ from one component to another. We can form the lattice  $L$  of  $\vec{\psi}$  by taking all integral linear combinations of wave vectors appearing in the union  $\cup_\alpha L_\alpha$ .

In Fourier space the condition (A3) for the indistinguishability of  $\vec{\psi}$  and  $\vec{\psi}'$  then requires that

$$\psi_{\alpha_1}(\mathbf{k}_1) \cdots \psi_{\alpha_j}(\mathbf{k}_j) \cdot \psi_{\alpha_{j+1}}^*(-\mathbf{k}_{j+1}) \cdots \psi_{\alpha_n}^*(-\mathbf{k}_n) = \psi'_{\alpha_1}(\mathbf{k}_1) \cdots \psi'_{\alpha_j}(\mathbf{k}_j) \cdot \psi'_{\alpha_{j+1}}^*(-\mathbf{k}_{j+1}) \cdots \psi'_{\alpha_n}^*(-\mathbf{k}_n) \quad (\text{A5})$$

whenever  $\mathbf{k}_1 + \cdots + \mathbf{k}_n = 0$ , for any choice of the components  $\alpha_1 \dots \alpha_n$  and of the indices  $j$  and  $n$ . For  $n=2$  and  $j=1,2$  this gives

$$\psi'_{\alpha_1}(\mathbf{k}) \psi'_{\alpha_2}^*(\mathbf{k}) = \psi_{\alpha_1}(\mathbf{k}) \psi_{\alpha_2}^*(\mathbf{k}), \quad (\text{A6})$$

$$\psi'_{\alpha_1}(\mathbf{k}) \psi'_{\alpha_2}(-\mathbf{k}) = \psi_{\alpha_1}(\mathbf{k}) \psi_{\alpha_2}(-\mathbf{k}). \quad (\text{A7})$$

When  $\alpha_1 = \alpha_2 = \alpha$  Eq. (A6) becomes

$$|\psi'_{\alpha}(\mathbf{k})|^2 = |\psi_{\alpha}(\mathbf{k})|^2, \quad (\text{A8})$$

which implies that the corresponding individual components of  $\vec{\psi}$  and  $\vec{\psi}'$  differ by only a phase:

$$\psi'_\alpha(\mathbf{k}) = e^{2\pi i \chi_\alpha(\mathbf{k})} \psi_\alpha(\mathbf{k}). \quad (\text{A9})$$

Equation (A7) (still with  $\alpha_1 = \alpha_2 = \alpha$ ) and the corresponding equation for the third-order correlation function  $\psi_\alpha(\mathbf{k}_1)\psi_\alpha(\mathbf{k}_2)\psi_\alpha(-\mathbf{k}_1-\mathbf{k}_2)$  then establish that  $\chi_\alpha(\mathbf{k})$  is linear on the lattice  $L_\alpha$  to within an additive integer and thus has all the usual properties of a gauge function, but only with regard to a single component of  $\vec{\psi}$ :

- (1) The equality (A5) for any higher-order correlation function constructed from a single component of  $\vec{\psi}$  is then ensured through the linearity of the corresponding gauge function.
- (2) Because the gauge function  $\chi_\alpha(\mathbf{k})$  is linear on the lattice  $L_\alpha$  it can be uniquely extended to all of  $L_\alpha$  to cover points at which it cannot be inferred from Eq. (A9) because  $\psi_\alpha(\mathbf{k})=0$ .
- (3) It is only necessary to specify the values of  $\chi_\alpha$  on a set of generating vectors of  $L_\alpha$  in order to specify it everywhere on  $L_\alpha$ .

Next we use Eqs. (A6) or (A7) together with Eq. (A9) to establish the identity

$$\chi_{\alpha_1}(\mathbf{k}) \equiv \chi_{\alpha_2}(\mathbf{k}) \quad (\text{A10})$$

for all wave vectors for which  $\psi_{\alpha_1}(\mathbf{k})$  and  $\psi_{\alpha_2}(\mathbf{k})$  are both nonzero. It then holds for all  $\mathbf{k}$  in  $L_{\alpha_1} \cap L_{\alpha_2}$  due to the unique linear extensions of  $\chi_{\alpha_1}(\mathbf{k})$  and  $\chi_{\alpha_2}(\mathbf{k})$  over these lattices. Because any two gauge functions are equal on the intersection of their lattices of definition we can define a single function  $\chi(\mathbf{k})$  on the union  $\cup_\alpha L_\alpha$  as

$$\chi(\mathbf{k}) = \begin{cases} \chi_{\alpha_1}(\mathbf{k}) & \text{if } \mathbf{k} \in L_{\alpha_1}, \\ \chi_{\alpha_2}(\mathbf{k}) & \text{if } \mathbf{k} \in L_{\alpha_2}, \\ \vdots & \vdots \end{cases} \quad (\text{A11})$$

By definition,  $\chi(\mathbf{k})$  is linear over each individual lattice  $L_\alpha$ . We now show that  $\chi(\mathbf{k})$  can be linearly extended over the whole of  $L$  (which is the set of all integral linear combinations of vectors in  $\cup_\alpha L_\alpha$ ), such that

$$\chi(\mathbf{k}_1 + \mathbf{k}_2) \equiv \chi(\mathbf{k}_1) + \chi(\mathbf{k}_2), \quad \mathbf{k}_1 \in L_{\alpha_1}, \mathbf{k}_2 \in L_{\alpha_2}. \quad (\text{A12})$$

This is the case if for every linearly dependent set of wave vectors

$$\mathbf{k}_1 + \mathbf{k}_2 + \dots + \mathbf{k}_n = 0, \quad \mathbf{k}_1 \in L_{\alpha_1} \dots \mathbf{k}_n \in L_{\alpha_n}, \quad (\text{A13})$$

the value of  $\chi(\mathbf{k}_1 + \mathbf{k}_2 + \dots + \mathbf{k}_n)$ , which by Eqs. (A12) and (A11) is equal to  $\chi_{\alpha_1}(\mathbf{k}_1) + \chi_{\alpha_2}(\mathbf{k}_2) + \dots + \chi_{\alpha_n}(\mathbf{k}_n)$ , necessarily vanishes. This requirement is indeed satisfied due to the equality of the correlation functions,

$$\begin{aligned} & \psi_{\alpha_1}(\mathbf{k}_1)\psi_{\alpha_2}(\mathbf{k}_2)\dots\psi_{\alpha_n}(\mathbf{k}_n) \\ &= \psi'_{\alpha_1}(\mathbf{k}_1)\psi'_{\alpha_2}(\mathbf{k}_2)\dots\psi'_{\alpha_n}(\mathbf{k}_n). \end{aligned} \quad (\text{A14})$$

Thus a single function  $\chi(\mathbf{k})$ , linear on the whole of  $L$ , serves as one gauge function relating all the components

of two indistinguishable multicomponent fields as shown in Eq. (A2). The existence of this gauge function ensures that condition (A5) is satisfied for any other possible correlation function.

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