Physical applications of crystallographic color groups: Landau theory of phase transitions

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The simplest crystallographic color groups are the permutational color groups. Elements of these groups combine two types of transformations: One is a rotation and/or translation of physical space and the other is a permutation. The groups considered here are subgroups of direct products and abstractly isomorphic to crystallographic groups, hence their relative simplicity. Despite this simplicity, there is a richness of information contained in each such group. The group symbol $G^P \equiv G/H'/H\ (A,A')_n$ conveys the following: the isomorphic crystallographic group G, a subgroup H' of G, the largest normal subgroup H of G, contained in H', and a transitive group of permutations $P \equiv (A,A')_n$ isomorphic to the factor group G/H. We derive and tabulate here all classes of equivalent permutational color point groups using a definition of equivalence classes which we physically motivate. For applications we require and report here the permutation representation $D_G^{H'}$ of G associated with each G^P and we reduce $D_G^{H'}$ into irreducible components. The major application given here is to the Landau theory of symmetry change in continuous phase transitions. A complete set of tables is presented for all allowed equitranslational ("Zellengleich" or $k=0$) phase transitions in crystals based on group-theoretical criteria, including a new "kernel-core" criterion. The tables may be used to determine all active representations for transitions between two specific groups or alternatively, all possible subgroups which can be obtained from a specific group and irreducible representation. We also relate two classifications schemes for phase transitions to the structure of permutational color groups.

I. INTRODUCTION

In many problems in solid state physics it is necessary to determine relationships between the symmetry group of a crystal and its subgroups, and between the representations of the symmetry group and representations of its subgroups and factor groups.[1–4]

We present four examples: In the Landau theory of phase transitions[3] the symmetry group H' of the lower-symmetry phase is a subgroup of the symmetry group G of the higher-symmetry phase. In this theory, when applying the chain subduction criterion,[5–8] one determines the number of times the identity representation $D_{H'}^1$ of each subgroup H' of a space group G is contained in the restriction of an irreducible representation D_G^j of G to the subgroup H'. In lattice vibrational problems one needs the irreducible representations of the symmetry group G of the crystal whose basis functions are combinations of the linearly independent displacements of the atoms.[2,4,9] These irreducible representations are contained in the direct product of the polar vector representation D_G^V and the permutation representation D_G^{perm} of the atomic positions. These irreducible representations are also of importance in determining the existence of the Jahn-Teller effect.[10,11]

In classifying all possible magnetic arrangements on crystals one can use magnetic space groups[12,13] or other types of color groups.[14,15] One can also determine the irreducible representations of the nonmagnetic symmetry group of the crystal whose basis functions, the magnetic modes, are linear combinations of the components of the atomic spins.[15–19] These are the irreducible representations contained in the direct product of the axial vector representation D_G^A and the permutation representation D_G^{perm} of the magnetic atoms.

All relationships between groups, their subgroups and factor groups, and their representations which are required in solving such problems can be determined, as we shall show, from the theory of permutational crystallographic color groups. Permutational crystallographic color groups are a special type of a general class of groups called "color groups"[20,21] or "metacrystallographic groups."[22]

Color groups are generalizations of the classical crystallographic groups. The elements of these groups consist of elements of classical crystallographic groups combined with some additional operator. A general theory of crystallographic color groups has been given by Koptsik and Kotzev[20,23] and has been the topic of some recent reviews.[14,21,24,25] Well-known special cases of color groups are magnetic groups[12,13] and spin groups.[26–33] These and other types of color groups[14,15] have been used in the classification of magnetic arrangements in crystals, of crystals with defects,[21] and incommensurate crystals.[34–36] Permutational color point groups and many of the permutational color space groups have been tabulated.[37–44] It is the purpose of this paper to demonstrate the applicability of the theory and tables of these groups to problems in solid-state physics.

In Sec. II we briefly discuss the mathematical structure of crystallographic color groups and we give a method of deriving one type of such groups, the so-called permutational color groups. Examples are given which show that magnetic groups and black and white groups are special cases of crystallographic color groups.

In Sec. III we discuss properties of permutational crystallographic color groups. We choose a definition of equivalence classes of permutational crystallographic color groups based on physical reasons which is different from that used by previous authors.[20,37,38,40] We then tabulate all permutational crystallographic color point groups. In Sec. IV we demonstrate that the permutation representation associated with each permutational color group can be considered as both an "induced" or an "engendered" representation. Some useful properties of induced and engendered representations are given. The decomposition of the permutation representation associated with each permutational crystallographic color point group is then tabulated.

The group-theoretical criteria used in the analysis of continuous phase transitions based on the Landau theory are reformulated in Sec. V in terms of the theory of permutational crystallographic color groups. It is shown that such a reformulation, along with the tables given here, simplifies the application of these criteria. Two classification schemes of phase transitions based on the theory of permutational crystallographic color groups are discussed in Sec. VI.

II. CRYSTALLOGRAPHIC COLOR GROUPS

Let G be a crystallographic group with elements $g \in G$ and P an arbitrary group with elements $p \in P$. A crystallographic color group G^P belonging to the family of G and P is:

(1) A set of pairs $\langle p;g \rangle$ where all elements $g \in G$ appear as right-hand-side components of members of the set, and all elements $p \in P$ appear as left-hand-side components.

(2) A composition law is defined such that the product of any two members of the set is contained in the set, and that the group axioms[1] are satisfied.

The many and varied crystallographic color groups can be distinguished by either the particular group P or the specific composition law used. Using group-extension theory, it has been shown[14,20,23,24] that depending on the composition law there are four types of color symmetry groups P-type, Q-type, W_P-type, and W_Q-type groups. The composition law is, respectively, determined by the direct product, semidirect product, wreath product, and generalized wreath product of the groups P and G.[14,21,24]

The group G is a crystallographic group and groups P have been chosen primarily on the basis of the application of color groups as symmetry groups of functions.[22,25] In physical applications, the functions represent physical properties defined on the atoms of a crystal. Examples of groups P are abstract groups,[42] the time-inversion group,[12,13] groups of matrices,[43] groups of permutations,[38,44,45] and groups of rotations and antirotations.[26–32]

In this paper we shall restrict ourselves to physical applications of P-type crystallographic color groups G^P which are isomorphic to G, i.e., $G^P \simeq G$. As all P-type color groups G^P are subgroups of the direct product $P \times G$, the composition law for elements $\langle p_i;g_i \rangle \in G^P$ is given by

$$\langle p_1;g_1 \rangle \langle p_2;g_2 \rangle = \langle p_1 p_2; g_1 g_2 \rangle \ . \tag{1}$$

The identity element is $\langle e_P;e_G \rangle$ where e_P is the identity element of P and e_G of G. The inverse of an element $\langle p_i;g_i \rangle$ is

$$\langle p_i;g_i \rangle^{-1} = \langle p_i^{-1};g_i^{-1} \rangle \ .$$

A. Isomorphism theorem for P-type groups

A method which can be used to derive all P-type color groups belonging to a family of G and P is based on an isomorphism theorem[46] and is given for the general case by Zamorzaev.[45] For P-type color groups G^P isomorphic to a crystallographic group G the method is as follows: Let $G^P=\{\langle p_i;g_i\rangle\}\simeq G$ be a group belonging to the family of G and P and isomorphic to the group G. Let $H^{(1)}$ be the subgroup of G^P of all elements of the form $\langle e_P;h\rangle, h\in H\subset G$. It follows from Eq. (1) and the assumed isomorphism $G^P\simeq G$ that $H^{(1)}$ is a normal subgroup of $G^P, H^{(1)}\lhd G^P$. Therefore $H\lhd G$ and the factor groups $G^P/H^{(1)}$ and G/H are isomorphic to the group P:

$$G^P/H^{(1)}\simeq G/H\simeq P\ . \tag{2}$$

Using the isomorphisms of Eq. (2) one constructs all P-type color groups $G^P\simeq G$ belonging to the family of G and P as follows: First, one finds all normal subgroups H of G such that G/H is isomorphic to P. For each normal subgroup $H\lhd G$ and each isomorphism $G/H\simeq P$, G is written in a coset decomposition with respect to H, and P written as

$$\begin{aligned} G&=H+g_2H+\cdots+g_nH\ ,\\ P&=e_P+P_2+\cdots+P_n\ , \end{aligned} \tag{3}$$

where each coset g_iH, considered as the ith element of the factor group G/H, and each element p_i of P, for $i=1,2,\ldots,n$, are mapped into each other by the isomorphism $G/H\simeq P$. One then pairs the element p_i of P with each element g_ih of the ith coset g_iH of G to form pairs $\langle p_i;g_ih\rangle$. The P-type color group $G^P\simeq G$ can be written as a union of cosets

$$\langle p_i;g_i\rangle H^{(1)}=\{\langle p_i;g_ih\rangle, h\in H\}\ .$$

We have

$$G^P=H^{(1)}+\langle p_2;g_2\rangle H^{(1)}+\cdots+\langle p_n;g_n\rangle H^{(1)}\ . \tag{4}$$

B. Examples of P-type groups

We present some well-known examples of P-type crystallographic color point groups G^P isomorphic to G. We first consider a group belonging to the family of the crystallographic point group $G=D_3$ and $P=1'=\{1,1'\}$, where $1'$ is time inversion.[22] To construct a group with $G/H\simeq P$ we take $H=C_3$ and write Eq. (3) as

$$\begin{aligned} G&=C_3+2_xC_3\ ,\\ P&=1+1'\ . \end{aligned} \tag{5}$$

The pairing of the elements of the cosets of G with elements of P means in this case that each element p_i of P is paired with each of three elements of G. The first element $p_1=1$ is paired with each of the three elements of the first coset of G, i.e., the three elements of the subgroup $H=C_3=\{1,3_z,3_z^2\}$. This pairing gives the three elements of the subgroup $H^{(1)}$ of G^P:

$$C_3^{(1)}=\{\langle 1;1\rangle,\langle 1;3_z\rangle,\langle 1;3_z^2\rangle\}\ . \tag{6}$$

Pairing of the second element $p_2=1'$ with the elements of the second coset $2_xC_3=\{2_x,2_y,2_{xy}\}$ gives the additional three elements:

$$\langle 1';2_x\rangle C_3^{(1)}=\{\langle 1';2_x\rangle,\langle 1';2_y\rangle,\langle 1';2_{xy}\rangle\}\ . \tag{7}$$

This color group, containing six elements, is written in the notation of Eq. (4) as

$$G^P=C_3^{(1)}+\langle 1';2_x\rangle C_3^{(1)}\ . \tag{8}$$

This group is one of the 58 nontrivial magnetic point groups,[2] $D_3(C_3)=32'$ and also one of the 598 spin point groups,[30,33] $3^{(1)}2^{(1')}$.

A second example of a P-type crystallographic color point group with the same mathematical structure but with a different group P, is the group belonging to the family of $G=D_3$ and $P=S_2=\{(1)(2),(12)\}$, the permutation group of two objects. Again taking $H=C_3$, the color group $G^P\simeq G$ consists of six elements similar to those listed in Eqs. (6) and (7). In those equations the left-hand-side component 1 is replaced by the permutation (1)(2), and $1'$ by the permutation (12). This group belongs to a class of color groups which has been called "black and white" or "two-color" groups.[13,37,38]

As a final example we take $G=D_3$ and

$$\begin{aligned} P=S_3=\{&(1)(2)(3),(123),(132)\ ,\\ &(1)(23),(13)(2),(12)(3)\}\ . \end{aligned}$$

Taking $H=C_1$ we have $G\simeq P$. One isomorphism of G onto P leads to the three-color group consisting of the six elements[37,40,44]:

$$\begin{aligned} &\langle (1)(2)(3);1\rangle\ ,\quad \langle (1)(23);2_x\rangle\ ,\\ &\langle (123);3_z\rangle\ ,\quad \langle (13)(2);2_y\rangle\ ,\\ &\langle (132);3_z^2\rangle\ ,\quad \langle (12)(3);2_{xy}\rangle\ . \end{aligned} \tag{9}$$

The last two examples were of groups belonging to a type of crystallographic color groups called permutational crystallographic color groups. Permutational crystallographic color groups are the topic of the following section.

III. PERMUTATIONAL COLOR GROUP

We consider here P-type crystallographic color groups, G^P isomorphic to G, belonging to a family of G and P, where G is a crystallographic group and P a transitive group of permutations. We shall call these groups "permutational color groups."

All permutational color groups can be derived using Zamorzaev's method[45] given in the preceding section by taking P as a transitive group of permutations. A second method for deriving all permutational color groups has been given by van der Waerden and Burckhardt[44] based on the theory of transitive permutation representations of a group G.[46] It has been shown[20] that a combination of both methods significantly simplifies the derivation of these groups.

We first define transitive permutation representations of a group G and briefly review the method of van der Waerden and Burckhardt. We then present the combined method of constructing permutational color groups. Finally we give the definition of equivalence classes of permutational color groups which we shall use.

A. Transitive permutation representations of G

Let H' be an arbitrary subgroup of G of finite index $n=[G:H']$. For each subgroup H' of finite index there exists[46] a subgroup H of H' which is the maximal normal subgroup of G contained in H'. The group H is called the "core" of H', $\text{core}H' \equiv H$, and is defined as the intersection of all subgroups conjugate to H' by elements of G:

$$\text{core}H' \equiv \bigcap_{g \in G} gH'g^{-1} \equiv H \ . \tag{10}$$

If it can be proven that there is a homomorphism $\pi_G^{H'}$,

$$\pi_G^{H'}:\ G \to P \subseteq S_n \ , \tag{11a}$$

$$P \simeq G/H \ , \tag{11b}$$

of the group G onto a transitive group of permutations P which is a subgroup of the symmetric group S_n. P is isomorphic to the factor group G/H and the normal subgroup $H \equiv \text{core}H'$ is the kernel of the homomorphism. Under this homomorphism the subgroup H' of G is mapped onto a subgroup P' of P:

$$\pi_G^{H'}:\ H' \to P' \subset P \ , \tag{12a}$$

$$P' \simeq H'/H \subset G/H \ . \tag{12b}$$

The $\text{core}P' = e_P \simeq C_1$.

The homomorphism $\pi_G^{H'}$ defined by Eq. (11a) determines the transitive permutation representation $\Pi_G^{H'}$ of G generated by the subgroup H':

$$\Pi_G^{H'} = \{\pi_G^{H'}(g); g \in G\} \ . \tag{13}$$

The kernel of this representation, the set of all $g \in G$ mapped by $\Pi_G^{H'}$ onto the identity permutation $e_P \in P$, is the subgroup $H \equiv \text{core}H'$ defined by Eq. (10). We have

$$\ker \Pi_G^{H'} = \text{core}H' \equiv H \ . \tag{14}$$

This transitive permutation representation of G is constructed as follows: One writes the coset decomposition of G with respect to H':

$$G = H' + g_2H' + \cdots + g_nH' \ . \tag{15}$$

An element $g \in G$ is mapped by the homorphism $\pi_G^{H'}$ into a permutation denoted by $\pi_G^{H'}(g)$ and defined as the permutation of the indices $i=1,2,\ldots,n$ of the cosets g_iH' of the coset decomposition equation (15). Under the action of $g \in G$, from the left, each coset g_iH' is transformed into the coset gg_iH';

$$\pi_G^{H'}(g) = \begin{bmatrix} H' & g_2H' & \cdots & g_nH' \\ gH' & gg_2H' & \cdots & gg_nH' \end{bmatrix} \simeq p \in P \ . \tag{16}$$

The right-hand side of Eq. (16) is a permutation $p \in P$. The image of the representation $\Pi_G^{H'}, \text{Im}\Pi_G^{H'}$, is the set of all distinct permutations $\pi_G^{H'}(g)$ in the representation $\Pi_G^{H'}$ defined in Eq. (13). This set constitutes a transitive group of permutations which is a subgroup of the symmetric group S_n, that is $\text{Im}\Pi_G^{H'} = P \subset S_n$.

B. Construction of permutational color groups

One can construct all permutational color groups using the method of van der Waerden and Burckhardt[44]: First one chooses a subgroup H' of G and constructs the permutation representation $\Pi_G^{H'}$ of G generated by the subgroup H' using Eq. (16). One then pairs each element $g \in G$ with the permutation $\pi_G^{H'}(g) = p \in P$ to construct a set of pairs $\langle \pi_G^{H'}(g); g \rangle = \langle p; g \rangle$. Because $\Pi_G^{H'}$ is a representation of G,

$$\pi_G^{H'}(g_1)\pi_G^{H'}(g_2)=\pi_G^{H'}(g_1g_2) ,$$

and the composition law for the set of pairs is the same as Eq. (1):

$$\langle \pi_G^{H'}(g_1);g_1\rangle\langle \pi_G^{H'}(g_2);g_2\rangle=\langle \pi_G^{H'}(g_1g_2);g_1g_2\rangle . \tag{17}$$

Therefore, this set of pairs constitutes a permutational color group G^P isomorphic to G belonging to the family of G and P. The group $P=\mathrm{Im}\Pi_G^{H'}$ is the transitive group of permutations isomorphic to $G^P/H^{(1)}\simeq G/H$ where $H=\mathrm{core}H'$. To find all permutational color groups $G^P\simeq G$ one could repeat the above procedure for each subgroup H' of all groups G.

However, Koptsik and Kotzev[20] have generalized Zamorzaev's method[45] in such a manner that it is not always necessary to repeat the above procedure for each subgroup H' of all groups G. Two abstract groups A and A' are introduced to accomplish this: Let H' be a subgroup of G with $\mathrm{core}H'=H$. There exist two abstract groups A and A' such that

$$A\simeq G/H ,$$
$$A'\simeq H'/H , \tag{18}$$

and such that A' is a subgroup of A. The permutation representation $\Pi_A^{A'}$ of A constructed using Eq. (16),

$$\Pi_A^{A'}=\{\pi_A^{A'}(a);a\in A\} , \tag{19}$$

is a faithful representation of A. We have from Eqs. (11), (13), and (18) that $\mathrm{Im}\Pi_A^{A'}\simeq\mathrm{Im}\Pi_G^{H'}$, and that

$$\pi_G^{H'}(g_ih)=\pi_A^{A'}(a_i) \tag{20}$$

for all $h\in H$. Note that g_ih is an element of the coset g_iH of G which is isomorphic by Eq. (18) to the element a_i of A. From Eqs. (17) and (20) it follows that the elements of the permutational color group G^P constructed from G and H' satisfy

$$\langle p_i;g_ih\rangle=\langle \pi_G^{H'}(g_ih);g_ih\rangle=\langle \pi_A^{A'}(a_i);g_ih\rangle \tag{21}$$

for all $h\in H=\mathrm{core}H'$.

Consequently, all permutational color groups $G^P\simeq G$ derived from all groups G and H' having the same groups A and A' defined by Eq. (18), can be constructed from the same permutation representation $\Pi_A^{A'}$ of A using Eq. (21). One then needs only to construct the faithful transitive permutation $\Pi_A^{A'}$ of $A\simeq G/H$. We shall denote by the symbol $(A,A')_n$ the transitive group of permutation $P\subset S_n$ isomorphic to A and identical to $\mathrm{Im}\Pi_A^{A'}$,

$$P\equiv\mathrm{Im}\Pi_A^{A'}\equiv(A,A')_n\simeq A .$$

The subindex n is the index of the subgroup A' in A, H' in G, of P' in P, and is equal to the dimensions of the permutation representations $\Pi_A^{A'}$ and $\Pi_G^{H'}$, denoted by $\dim\Pi_A^{A'}$ and $\dim\Pi_G^{H'}$, respectively. When $A'=\{e_A\}\simeq C_1$ we shall use the symbol $(A)_n$ in place of $(A,C_1)_n$. In this case $(A)_n=\mathrm{Im}\Pi_A^{C_1}$ where $\Pi_A^{C_1}$ is the regular representation of the abstract group A.

Each permutational color group $G^P\simeq G$ belonging to a family of G and P is uniquely determined by G and the subgroup H' of G. This has led to the symbol[25] $G(H')$ for these groups. However, this symbol may be misinterpreted as a symbol of a magnetic group.[1,2]

We propose, instead, a new more explicit notation for these groups. This notation[37–40] $G/H'/H$ includes explicitly the normal subgroup H of G such that $G/H\simeq P$ and $\mathrm{core}H'=H\simeq H^{(1)}$, see Eqs. (2) and (10). We shall use the notation[20] $G/H'/H$ $(A,A')_n$ which includes explicitly a symbol for the transitive group of permutation $P=(A,A')_n$. This notation is useful in that two permutational color groups G^P having in this notation the same symbol $(A,A')_n$ belong to families with the same transitive permutation group P. This notation also provides information useful in the classifications[23,38] of the permutational color groups and, as will be shown in Sec. VI, in the classification of phase transitions.[47]. In the case where $H'=H$ and $A'\simeq C_1$ the notation G/H $(A)_n$ will be used instead of $G/H/H$ $(A,C_1)_n$.

The group notation $G^P=G/H'/H$ $(A,A')_n$ contains the following information:

$$G\simeq G^P\equiv\{\langle p;g\rangle;g\in G,p\in P\} , \tag{22a}$$

$$H\simeq H^{(1)}$$
$$\equiv\{\langle e_P;h\rangle;h\in H\equiv\mathrm{Core}H'\} , \tag{22b}$$

$$H'\simeq(H')^{P'}$$
$$\equiv\{\langle p';h'\rangle;h'\in H',p'\in P'\subset P\} , \tag{22c}$$

$$(A,A')_n\equiv P\subseteq S_n , \tag{22d}$$

$$A\simeq P\simeq G/H\simeq G^P/H^{(1)} , \tag{22e}$$

$$A'\simeq P'\simeq H'/H\simeq(H')^{P'}/H^{(1)};A'\subset A , \tag{22f}$$

$$n=[A:A']=[P;P']=[G;H'] \\ =\dim\Pi_G^{H'}=\dim\Pi_A^{A'} . \quad (22g)$$

H is the normal subgroup of G whose elements are paired in G^P with the identity permutation $e_P \in P$. The transitive group of permutations $P=(A,A')_n$ is a subgroup of the symmetric group S_n and is defined, using Eqs. (16) and (18), by the representation $\Pi_A^{A'}$, Eq. (19).

The above method, using Eqs. (16) through (20), is quite general[20,23]: The groups G and H' can be either point groups or space groups. In the latter case H' can be either an equitranslational or equiclass subgroup of the space group G. For equitranslational subgroups H' of G, the common subgroup of translations is an invariant subgroup of G, H', and $H=\text{core}H'$. The factor groups $G/T \simeq \hat{G}, H'/T \simeq \hat{H}'$, and $H/T \simeq \hat{H}$ are isomorphic to the respective point groups $\hat{G}$, $\hat{H}'$, and $\hat{H}=\text{core}\hat{H}'$, of the corresponding space groups. In this case of equitranslational subgroups H', all permutational color space groups $G/H'/H\ (A,A')_n$ with the same permutational color point group $\hat{G}/\hat{H}'/\hat{H}\ (A,A')_n$ have the same group P. The permutation group

$$P=(A,A')_n \simeq G/H \simeq \hat{G}/\hat{H}$$

is the image of the permutation representation $\Pi_{\hat{G}}^{\hat{H}'}$ and of all $\Pi_G^{H'}$:

$$P=(A,A')_n=\text{Im}\Pi_A^{A'}=\text{Im}\Pi_G^{H'}=\text{Im}\Pi_{\hat{G}}^{\hat{H}'} . \quad (23)$$

For all point groups $\hat{G}$ and space groups G with equitranslational subgroups H', each factor group G/H' is isomorphic to one of 18 abstract groups. These are the 18 abstract groups to which all 32 point groups are isomorphic.[37] We shall denote each of these 18 abstract groups A, and subgroups A' of A, by a representative point group isomorphic to A. These 18 representative point groups are C_1, C_2, C_3, C_4, C_6, D_2, D_3, D_4, D_6, C_{4h}, C_{6h}, D_{2h}, D_{4h}, D_{6h}, T, T_h, O, and O_h. There are 45 transitive groups of permutation $(A,A')_n \subseteq S_n$ which are isomorphic to these 18 abstract groups A.[20,21] These 45 groups are used in a classification of all permutational color point groups[38] and, as we shall demonstrate below in Sec. V, for determining group-subgroup relationships in the theory of phase transitions.

C. Equivalence of permutational color groups

The problem of finding all permutational crystallographic color groups $G^P \simeq G$ can be solved by one of the methods given above. However, one usually does not want to know all such groups but only one from each equivalence class of permutational color groups. First, equivalence classes must be defined.

There is no general agreement on the definition of equivalence classes of these groups.[25] The definition of equivalence classes of permutational color groups which we shall use[25,44] has been chosen on the basis of the physical applications of these groups. It is a special case of the definition of equivalence classes[20,24] used for more general types of color groups:

The permutational color groups $G_1/H_1'/H_1$ and $G_2/H_2'/H_2$ belong to the same equivalence class and are said to be equivalent, if they belong to the same family $G_1=G_2=G$ and the subgroups H_1' and H_2' are conjugate subgroups in G. That is, there exists an element $g \in G$ such that $H_1' = gH_2'g^{-1}$.

It follows that two equivalent permutational color groups $G/H_1'/H_1$ and $G/H_2'/H_2$ are such that $H_1=H_2$. A list of one group from each equivalence class of all permutational color point groups $G^P \simeq G$ is given in Table I. The number of classes of G^P listed in this table, 279, is greater than the number, 244, in the tables of Refs. 20, 37, and 40. This is because in the definition of equivalence classes used in these references, H_1' and H_2' need only be conjugate subgroups of the full group of rotations O(3). This is a less stringent condition than the condition to be conjugate subgroups of G used in our definition.

Central in the physical applications of permutational color groups discussed in Secs. V and VI, is the matrix representation $D_G^{H'}$ associated with each permutational color group defined in Sec. IV. With our definition of equivalence classes, representations $D_G^{H'}$ corresponding to equivalent permutational color groups are equivalent representations, and representations corresponding to nonequivalent permutational color groups are nonequivalent representations.

IV. PERMUTATION REPRESENTATION $D_G^{H'}$

The matrix representation $D_G^{H'}$ associated with each permutational color group $G/H'/H\ (A,A')_n$ plays a central role in the physical applications of permutational color groups. This representation is defined as follows: To each permutation

TABLE I. List of all equivalence classes of permutational color point groups is given in the notation $\hat{G}/\hat{H}'/\hat{H}\ (A,A')_n$ or $\hat{G}/\hat{H}\ (A)_n$ when $\hat{H}'=\hat{H}$ and $A'=A$. Enumeration used consists of a number to the left of the decimal to denote the point group $\hat{G}$ in the numbering of Ref. 63, and a number or a number and letter to the right of the decimal. Equivalence classes with the same numbering and different letters are considered elsewhere (Refs. 20, 37, and 40) as the same equivalence class of permutational color point groups. Symbols Γ_ν denote the irreducible representations of the point group $\hat{G}$ in the notation of Ref. 63. Physically irreducible representations are enclosed in parentheses. A superindex s denotes that the irreducible representation is not Landau active. A superindex h denotes that the irreducible representation does not satisfy the Lifshitz homogeneity criterion. At the intersection of the column under Γ_ν and row alongside $\hat{G}/\hat{H}'/\hat{H}\ (A,A')_n$ is the coefficient $(D_{\hat{G}}^{H'} \mid \Gamma_\nu)$. An asterisk on this coefficient denotes that $\hat{H}'$ satisfies the chain subduction criterion for the transition between $\hat{G}$ and $\hat{H}'$ associated with the irreducible representation Γ_ν.

	C_1-1	${}^s\Gamma_1$
1.1	$C_1/C_1\ (C_1)_1$	1*

	$C_i-\bar{1}$		C_2-2		C_s-m	${}^s\Gamma_1$ / ${}^s\Gamma_1^+$	Γ_2 / Γ_1^-
2.1	$C_i/C_1\ (C_2)_2$	3.1	$C_2/C_1\ (C_2)_2$	4.1	$C_s/C_1\ (C_2)_2$	1	1*
2.2	$C_i/C_i\ (C_1)_1$	3.2	$C_2/C_2\ (C_1)_1$	4.2	$C_s/C_s\ (C_1)_1$	1*	

	$C_{2h}-2/m$		D_2-222		$C_{2v}-mm2$	${}^s\Gamma_1$ / ${}^s\Gamma_1^+$	Γ_2 / Γ_2^+	Γ_3 / Γ_1^-	Γ_4 / Γ_2^-
5.1	$C_{2h}/C_1\ (D_2)_4$	6.1	$D_2/C_1\ (D_2)_4$	7.1	$C_{2v}/C_1\ (D_2)_4$	1	1	1	1
5.2	$C_{2h}/C_s\ (C_2)_2$	6.2a	$D_2/C_2^x\ (C_2)_2$	7.3a	$C_{2v}/C_s^x\ (C_2)_2$	1			1*
5.3	$C_{2h}/C_2\ (C_2)_2$	6.2b	$D_2/C_2^z\ (C_2)_2$	7.2	$C_{2v}/C_2\ (C_2)_2$	1		1*	
5.4	$C_{2h}/C_i\ (C_2)_2$	6.2c	$D_2/C_2^y\ (C_2)_2$	7.3b	$C_{2v}/C_s^y\ (C_2)_2$	1	1*		
5.5	$C_{2h}/C_{2h}\ (C_1)_1$	6.3	$D_2/D_2\ (C_1)_1$	7.4	$C_{2v}/C_{2v}\ (C_1)_1$	1*			

	$D_{2h}-mmm$	${}^s\Gamma_1^+$	Γ_2^+	Γ_3^+	Γ_4^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-
8.1	$D_{2h}/C_1\ (D_{2h})_8$	1	1	1	1	1	1	1	1
8.2	$D_{2h}/C_i\ (D_2)_4$	1	1	1	1				
8.3a	$D_{2h}/C_2^y\ (D_2)_4$	1	1			1	1		
8.3b	$D_{2h}/C_2^z\ (D_2)_4$	1		1		1		1	
8.3c	$D_{2h}/C_2^x\ (D_2)_4$	1			1	1			1
8.4a	$D_{2h}/C_s^y\ (D_2)_4$	1	1					1	1
8.4b	$D_{2h}/C_s^z\ (D_2)_4$	1		1			1		1
8.4c	$D_{2h}/C_s^x\ (D_2)_4$	1			1		1	1	
8.5a	$D_{2h}/C_{2v}^x\ (C_2)_2$	1							1*
8.5b	$D_{2h}/C_{2v}^z\ (C_2)_2$	1						1*	
8.5c	$D_{2h}/C_{2v}^y\ (C_2)_2$	1					1*		
8.6	$D_{2h}/D_2\ (C_2)_2$	1				1*			
8.7a	$D_{2h}/C_{2h}^x\ (C_2)_2$	1			1*				
8.7b	$D_{2h}/C_{2h}^z\ (C_2)_2$	1		1*					
8.7c	$D_{2h}/C_{2h}^y\ (C_2)_2$	1	1*						
8.8	$D_{2h}/D_{2h}\ (C_1)_1$	1*							

TABLE I. (*Continued.*)

	C_4-4		$S_4-\bar{4}$	${}^s\Gamma_1$	Γ_2	$(\Gamma_3$	$\Gamma_4)^h$
9.1	$C_4/C_1\ (C_4)_4$	10.1	$S_4/C_1\ (C_4)_4$	1	1	1*	1*
9.2	$C_4/C_2\ (C_2)_2$	10.2	$S_4/C_2\ (C_2)_2$	1	1*		
9.3	$C_4/C_4\ (C_1)_1$	10.3	$S_4/S_4\ (C_1)_1$	1*			

	$C_{4h}-4/m$	${}^s\Gamma_1^+$	Γ_2^+	$(\Gamma_3^+$	$\Gamma_4^+)$	Γ_1^-	Γ_2^-	$(\Gamma_3^-$	$\Gamma_4^-)$
11.1	$C_{4h}/C_1\ (C_{4h})_8$	1	1	1	1	1	1	1	1
11.2	$C_{4h}/C_2\ (D_2)_4$	1	1			1	1		
11.3	$C_{4h}/C_m\ (C_4)_4$	1	1					1*	1*
11.4	$C_{4h}/C_i\ (C_4)_4$	1	1	1*	1*				
11.5	$C_{4h}/S_4\ (C_2)_2$	1					1*		
11.6	$C_{4h}/C_4\ (C_2)_2$	1				1*			
11.7	$C_{4h}/C_{2h}\ (C_2)_2$	1	1*						
11.8	$C_{4h}/C_{4h}\ (C_1)_1$	1*							

	D_4-422		$C_{4v}-4mm$		$D_{2d}-\bar{4}2m$	${}^s\Gamma_1$ / ${}^s\Gamma_1$	Γ_2 / Γ_2	Γ_3 / Γ_3	Γ_4 / Γ_4	Γ_5^h / Γ_5
12.1	$D_4/C_1\ (D_4)_8$	13.1	$C_{4v}/C_1\ (D_4)_8$	14.1	$D_{2d}/C_1\ (D_4)_8$	1	1	1	1	2*
12.2a	$D_4/C_2^x/C_1\ (D_4,C_2^x)_4$	13.2a	$C_{4v}/C_s^x/C_1\ (D_4,C_2^x)_4$	14.2	$D_{2d}/C_2^x/C_1\ (D_4,C_2^x)_4$	1		1		1*
12.2b	$D_4/C_2^{xy}/C_1\ (D_4,C_2^x)_4$	13.2b	$C_{4v}/C_s^{xy}/C_1\ (D_4,C_2^x)_4$	14.3	$D_{2d}/C_s^{xy}/C_1\ (D_4,C_2^x)_4$	1			1	1*
12.3	$D_4/C_2^z\ (D_2)_4$	13.3	$C_{4v}/C_2^z\ (D_2)_4$	14.4	$D_{2d}/C_2^z\ (D_2)_4$	1	1	1	1	
12.4a	$D_4/D_2^{(z,xy,\bar{x}y)}\ (C_2)_2$	13.4a	$C_{4v}/C_{2v}^{(z,xy,\bar{x}y)}\ (C_2)_2$	14.5	$D_{2d}/C_{2v}\ (C_2)_2$	1			1*	
12.4b	$D_4/D_2^{(z,x,y)}\ (C_2)_2$	13.4b	$C_{4v}/C_{2v}^{(z,x,y)}\ (C_2)_2$	14.6	$D_{2d}/D_2\ (C_2)_2$	1		1*		
12.5	$D_4/C_4\ (C_2)_2$	13.5	$C_{4v}/C_4\ (C_2)_2$	14.7	$D_{2d}/S_4\ (C_2)_2$	1	1*			
12.6	$D_4/D_4\ (C_1)_1$	13.6	$C_{4v}/C_{4v}\ (C_1)_1$	14.8	$D_{2d}/D_{2d}\ (C_1)_1$	1*				

	$D_{4h}-4/mmm$	${}^s\Gamma_1^+$	Γ_1^-	Γ_2^+	Γ_2^-	Γ_3^+	Γ_3^-	Γ_4^+	Γ_4^-	Γ_5^+	Γ_5^-
15.1	$D_{4h}/C_1\ (D_{4h})_{16}$	1	1	1	1	1	1	1	1	2	2
15.2a	$D_{4h}/C_2^x/C_1\ (D_{4h},C_2^x)_8$	1	1			1	1			1	1
15.2b	$D_{4h}/C_2^{xy}/C_1\ (D_{4h},C_2^x)_8$	1	1					1	1	1	1
15.3a	$D_{4h}/C_s^x/C_1\ (D_{4h},C_2^x)_8$	1			1	1			1	1	1
15.3b	$D_{4h}/C_s^{xy}/C_1\ (D_{4h},C_2^x)_8$	1			1		1	1		1	1
15.4	$D_{4h}/C_s^z\ (D_4)_8$	1		1		1		1			2*
15.5a	$D_{4h}/C_{2v}^x/C_s\ (D_4,C_2^x)_4$	1				1					1*
15.5b	$D_{4h}/C_{2v}^{xy}/C_s\ (D_4,C_2^x)_4$	1						1			1*
15.6	$D_{4h}/C_i\ (D_4)_8$	1		1		1		1		2*	
15.7a	$D_{4h}/C_{2h}^x/C_i\ (D_4,C_2^x)_4$	1				1				1*	
15.7b	$D_{4h}/C_{2h}^{xy}/C_i\ (D_4,C_2^x)_4$	1						1		1*	
15.8	$D_{4h}/C_2^z\ (D_{2h})_8$	1	1	1	1	1	1	1	1		

TABLE I. (*Continued.*)

	$D_{4h}-4/mmm$	${}^s\Gamma_1^+$	Γ_1^-	Γ_2^+	Γ_2^-	Γ_3^+	Γ_3^-	Γ_4^+	Γ_4^-	Γ_5^+	Γ_5^-
15.9	$D_{4h}/C_{2h}^z\ (D_2)_4$	1		1		1		1			
15.10a	$D_{4h}/D_2^{(z,x,y)}\ (D_2)_4$	1	1			1	1				
15.10b	$D_{4h}/D_2^{(z,xy,\bar{x}y)}\ (D_2)_4$	1	1					1	1		
15.11a	$D_{4h}/C_{2v}^{(z,x,y)}\ (D_2)_4$	1			1	1			1		
15.11b	$D_{4h}/C_{2v}^{(z,xy,\bar{x}y)}\ (D_2)_4$	1			1		1	1			
15.12	$D_{4h}/C_4\ (D_2)_4$	1	1	1	1						
15.13	$D_{4h}/S_4\ (D_2)_4$	1		1			1		1		
15.14a	$D_{4h}/D_{2d}^{(z,xy,\bar{x}y)}\ (C_2)_2$	1							1*		
15.15a	$D_{4h}/D_{2h}^{(z,xy,\bar{x}y)}\ (C_2)_2$	1						1*			
15.14b	$D_{4h}/D_{2d}^{(z,x,y)}\ (C_2)_2$	1					1*				
15.15b	$D_{4h}/D_{2h}^{(z,x,y)}\ (C_2)_2$	1				1*					
15.16	$D_{4h}/C_{4v}\ (C_2)_2$	1			1*						
15.17	$D_{4h}/C_{4h}\ (C_2)_2$	1		1*							
15.18	$D_{4h}/D_4\ (C_2)_2$	1	1*								
15.19	$D_{4h}/D_{4h}\ (C_1)_1$	1*									

	C_3-3	${}^s\Gamma_1$	$({}^s\Gamma_2$	${}^s\Gamma_3)^h$
16.1	$C_3/C_1\ (C_3)_3$	1	1*	1*
16.2	$C_3/C_3\ (C_1)_1$	1*		

			$C_{3v}-3m$	${}^s\Gamma_1$	Γ_2	${}^s\Gamma_3$
	D_3-32			${}^s\Gamma_1$	Γ_2	${}^s\Gamma_3^h$
18.1	$D_3/C_1\ (D_3)_6$	19.1	$C_{3v}/C_1\ (D_3)_6$	1	1	2*
18.2	$D_3/C_2/C_1\ (D_3,C_2)_3$	19.2	$C_{3v}/C_s/C_1\ (D_3,C_2)_3$	1		1*
18.3	$D_3/C_3\ (C_2)_2$	19.3	$C_{3v}/C_3\ (C_2)_2$	1	1*	
18.4	$D_3/D_3\ (C_1)_1$	19.4	$C_{3v}/C_{3v}\ (C_1)_1$	1*		

	$C_{6h}-6/m$	${}^s\Gamma_1^+$	Γ_4^+	Γ_1^-	Γ_4^-	$({}^s\Gamma_2^+$	${}^s\Gamma_3^+)$	$(\Gamma_5^+$	$\Gamma_6^+)$	$(\Gamma_2^-$	$\Gamma_3^-)$	$(\Gamma_5^-$	$\Gamma_6^-)$
23.1	$C_{6h}/C_1\ (C_{6h})_{12}$	1	1	1	1	1	1	1	1	1	1	1	1
23.2	$C_{6h}/C_s\ (C_6)_6$	1			1	1	1					1*	1*
23.3	$C_{6h}/C_2\ (C_6)_6$	1		1		1	1			1*	1*		
23.4	$C_{6h}/C_i\ (C_6)_6$	1	1			1	1	1*	1*				
23.5	$C_{6h}/C_{2h}\ (C_3)_3$	1				1*	1*						
23.6	$C_{6h}/C_3\ (D_2)_4$	1	1	1	1								
23.7	$C_{6h}/C_{3h}\ (C_2)_2$	1			1*								
23.8	$C_{6h}/C_6\ (C_2)_2$	1		1*									
23.9	$C_{6h}/C_{3i}\ (C_2)_2$	1	1*										
23.10	$C_{6h}/C_{6h}\ (C_1)_1$	1*											

TABLE I. (*Continued.*)

	$C_{3i}-\bar{3}$		C_6-6		$C_{3h}-\bar{6}$	$^s\Gamma_1$ $^s\Gamma_1$ $^s\Gamma_1^+$	$(^s\Gamma_2$ $(^s\Gamma_2$ $(^s\Gamma_2^+$	$^s\Gamma_3)$ $^s\Gamma_3)^h$ $^s\Gamma_3^+)$	Γ_4 Γ_4 Γ_1^-	$(\Gamma_5$ $(\Gamma_5$ $(\Gamma_2^-$	$\Gamma_6)$ $\Gamma_6)^h$ $\Gamma_3^-)$
17.1	$C_{3i}/C_1\ (C_6)_6$	21.1	$C_6/C_1\ (C_6)_6$	22.1	$C_{3h}/C_1\ (C_6)_6$	1	1	1	1	1*	1*
17.2	$C_{3i}/C_i\ (C_3)_3$	21.2	$C_6/C_2\ (C_3)_3$	22.2	$C_{3h}/C_s\ (C_3)_3$	1	1*	1*			
17.3	$C_{3i}/C_3\ (C_2)_2$	21.3	$C_6/C_3\ (C_2)_2$	22.3	$C_{3h}/C_3\ (C_2)_2$	1			1*		
17.4	$C_{3i}/C_{3i}\ (C_1)_1$	21.4	$C_6/C_6\ (C_1)_1$	22.4	$C_{3h}/C_{3h}\ (C_1)_1$	1*					

	$D_{3d}-\bar{3}m$		D_6-622		$C_{6v}-6mm$		$D_{3h}-\bar{6}m2$	$^s\Gamma_1$ $^s\Gamma_1$ $^s\Gamma_1^+$	Γ_2 Γ_2 Γ_2^+	Γ_3 Γ_3 Γ_1^-	Γ_4 Γ_4 Γ_2^-	Γ_6 $^s\Gamma_6^h$ $^s\Gamma_3^+$	Γ_5 Γ_5^h Γ_3^-
20.1	$D_{3d}/C_1\ (D_6)_{12}$	24.1	$D_6/C_1\ (D_6)_{12}$	25.1	$C_{6v}/C_1\ (D_6)_{12}$	26.1	$D_{3h}/C_1\ (D_6)_{12}$	1	1	1	1	2	2*
20.2	$D_{3d}/C_2/C_1\ (D_6,C_2^y)_6$	24.2a	$D_6/C_2^y/C_1\ (D_6,C_2^y)$	25.2a	$C_{6v}/C_s^y/C_1\ (D_6,C_2^y)_6$	26.2	$D_{3h}/C_2^y/C_1\ (D_6,C_2^y)_6$	1		1		1	1*
20.3	$D_{3d}/C_s/C_1\ (D_6,C_2^y)_6$	24.2b	$D_6/C_2^x/C_1\ (D_6,C_2^y)$	25.2b	$C_{6v}/C_s^x/C_1\ (D_6,C_2^y)_6$	26.3	$D_{3h}/C_s^x/C_1\ (D_6,C_2^y)_6$	1			1	1	1*
20.4	$D_{3d}/C_i\ (D_3)_6$	24.3	$D_6/C_2\ (D_3)_6$	25.3	$C_{6v}/C_2\ (D_3)_6$	26.4	$D_{3h}/C_s^z\ (D_3)_6$	1	1			2*	
20.5	$D_{3d}/C_{2h}/C_i\ (D_3,C_2)_3$	24.4	$D_6/D_2/C_2\ (D_3,C_2)_3$	25.4	$C_{6v}/C_{2v}/C_2\ (D_3,C_2)_3$	26.5	$D_{3h}/C_{2v}/C_s\ (D_3,C_2)_3$	1				1*	
20.6	$D_{3d}/C_3\ (D_2)_4$	24.5	$D_6/C_3\ (D_2)_4$	25.5	$C_{6v}/C_3\ (D_2)_4$	26.6	$D_{3h}/C_3\ (D_2)_4$	1	1	1	1		
20.7	$D_{3d}/C_{3v}\ (C_2)_2$	24.6a	$D_6/D_3^{(z,x,x')}\ (C_2)_2$	25.6a	$C_{6v}/C_{3v}^{(z,x,x')}\ (C_2)_2$	26.7	$D_{3h}/C_{3v}\ (C_2)_2$	1			1*		
20.8	$D_{3d}/D_3\ (C_2)_2$	24.6b	$D_6/D_3^{(z,y,y')}\ (C_2)_2$	25.6b	$C_{6v}/C_{3v}^{(z,y,y')}\ (C_2)_2$	26.8	$D_{3h}/D_3\ (C_2)_2$	1		1*			
20.9	$D_{3d}/C_{3i}\ (C_2)_2$	24.7	$D_6/C_6\ (C_2)_2$	25.7	$C_{6v}/C_6\ (C_2)$	26.9	$D_{3h}/C_{3h}\ (C_2)_2$	1	1*				
20.10	$D_{3d}/D_{3d}\ (C_1)_1$	24.8	$D_6/D_6\ (C_1)_1$	25.8	$C_{6v}/C_{6v}\ (C_1)$	26.10	$D_{3h}/D_{3h}\ (C_1)_1$	1*					

	$D_{6h}-6/mmm$	$^s\Gamma_1^+$	Γ_1^-	Γ_2^+	Γ_2^-	Γ_3^+	Γ_3^-	Γ_4^+	Γ_4^-	$^s\Gamma_6^+$	Γ_6^-	Γ_5^+	Γ_5^-
27.1	$D_{6h}/C_1\ (D_{6h})_{24}$	1	1	1	1	1	1	1	1	2	2	2	2
27.2a	$D_{6h}/C_2^x/C_1\ (D_{6h},C_2^x)_{12}$	1	1					1	1	1	1	1	1
27.2b	$D_{6h}/C_2^y/C_1\ (D_{6h},C_2^x)_{12}$	1	1			1	1			1	1	1	1
27.3a	$D_{6h}/C_s^x/C_1\ (D_{6h},C_2^x)_{12}$	1			1		1	1		1	1	1	1
27.3b	$D_{6h}/C_s^y/C_1\ (D_{6h},C_2^x)_{12}$	1			1	1			1	1	1	1	1
27.4	$D_{6h}/C_s\ (D_6)_{12}$	1		1			1		1	2			2*
27.5a	$D_{6h}/C_{2v}^x/C_s\ (D_6,C_2^x)_6$	1							1	1			1*
27.5b	$D_{6h}/C_{2v}^y/C_s\ (D_6,C_2^x)_6$	1					1			1			1*
27.6	$D_{6h}/C_i\ (D_6)_{12}$	1		1		1		1		2		2*	
27.7a	$D_{6h}/C_{2h}^x/C_i\ (D_6,C_2^x)_6$	1						1		1		1*	
27.7b	$D_{6h}/C_{2h}^y/C_i\ (D_6,C_2^x)_6$	1				1				1		1*	
27.8	$D_{6h}/C_2\ (D_6)_{12}$	1	1	1	1					2	2*		
27.9	$D_{6h}/D_2/C_2\ (D_6,C_2^x)_6$	1	1							1	1*		
27.10	$D_{6h}/C_{2v}/C_2\ (D_6,C_2^x)_6$	1			1					1	1*		
27.11	$D_{6h}/C_{2h}\ (D_3)_6$	1		1						2*			
27.12	$D_{6h}/D_{2h}/C_{2h}\ (D_3,C_2)_3$	1								1*			

TABLE I. (*Continued.*)

	$D_{6h}-6/mmm$	${}^s\Gamma_1^+$	Γ_1^-	Γ_2^+	Γ_2^-	Γ_3^+	Γ_3^-	Γ_4^+	Γ_4^-	${}^s\Gamma_6^+$	Γ_6^-	Γ_5^+	Γ_5^-
27.13	$D_{6h}/C_3\ (D_{2h})_8$	1	1	1	1	1	1	1	1				
27.14	$D_{6h}/C_{3i}\ (D_2)_4$	1		1		1		1					
27.15	$D_{6h}/C_6\ (D_2)_4$	1	1	1	1								
27.16	$D_{6h}/C_{3h}\ (D_2)_4$	1		1			1		1				
27.17a	$D_{6h}/D_3^{(z,x,x')}\ (D_2)_4$	1	1					1	1				
27.17b	$D_{6h}/D_3^{(z,y,y')}\ (D_2)_4$	1	1			1	1						
27.18a	$D_{6h}/C_{3v}^{(z,x,x')}\ (D_2)_4$	1			1		1	1					
27.18b	$D_{6h}/C_{3v}^{(z,y,y')}\ (D_2)_4$	1			1	1			1				
27.19a	$D_{6h}/D_{3h}^{(z,x,x')}\ (C_2)_2$	1							1*				
27.20a	$D_{6h}/D_{3d}^{(z,x,x')}\ (C_2)_2$	1						1*					
27.19b	$D_{6h}/D_{3h}^{(z,y,y')}\ (C_2)_2$	1					1*						
27.20b	$D_{6h}/D_{3d}^{(z,y,y')}\ (C_2)_2$	1				1*							
27.21	$D_{6h}/C_{6v}\ (C_2)_2$	1			1*								
27.22	$D_{6h}/C_{6h}\ (C_2)_2$	1		1*									
27.23	$D_{6h}/D_6\ (C_2)_2$	1	1*										
27.24	$D_{6h}/D_{6h}\ (C_1)_1$	1*											

	$T-23$	${}^s\Gamma_1$	$({}^s\Gamma_2$	${}^s\Gamma_3)$	${}^s\Gamma_4^h$
28.1	$T/C_1\ (T)_{12}$	1	1	1	3*
28.2	$T/C_2/C_1\ (T,C_2)_6$	1	1	1	1*
28.3	$T/C_3/C_1\ (T,C_3)_4$	1			1*
28.4	$T/D_2\ (C_3)_3$	1	1*	1*	
28.5	$T/T\ (C_1)_1$	1*			

	T_h-m3	${}^s\Gamma_1^+$	$({}^s\Gamma_2^+$	${}^s\Gamma_3^+)$	${}^s\Gamma_4^+$	Γ_1^-	$(\Gamma_2^-$	$\Gamma_3^-)$	Γ_4^-
29.1	$T_h/C_1\ (T_h)_{24}$	1	1	1	3	1	1	1.	3*
29.2	$T_h/C_s/C_1\ (T_h,C_s)_{12}$	1	1	1	1				2*
29.3	$T_h/C_2/C_1\ (T_h,C_2)_{12}$	1	1	1	1	1	1	1	1
29.4	$T_h/C_3/C_1\ (T_h,C_3)_8$	1			1	1			1*
29.5	$T_h/C_{2v}/C_1\ (T_h,C_{2v})_6$	1	1	1					1*
29.6	$T_h/D_2\ (C_6)_6$	1	1	1		1	1*	1*	
29.7	$T_h/T\ (C_2)_2$	1				1*			
29.8	$T_h/C_i\ (T)_{12}$	1	1	1	3*				
29.9	$T_h/C_{2h}/C_i\ (T,C_2)_6$	1	1	1	1*				
29.10	$T_h/C_{3i}/C_i\ (T,C_3)_4$	1			1*				
29.11	$T_h/D_{2h}\ (C_3)_3$	1	1*	1*					
29.12	$T_h/T_h\ (C_1)_1$	1*							

TABLE I. (*Continued.*)

	$O-432$		$T_d-\bar{4}3m$	$^s\Gamma_1$ / $^s\Gamma_1$	Γ_2 / Γ_2	$^s\Gamma_3$ / $^s\Gamma_3$	Γ_4 / Γ_4^h	$^s\Gamma_5$ / $^s\Gamma_5^h$
30.1	$O/C_1\ (O)_{24}$	31.1	$T_d/C_1\ (O)_{24}$	1	1	2	3*	3*
30.2	$O/C_2^z/C_1\ (O,C_2^z)_{12}$	31.2	$T_d/C_2/C_1\ (O,C_2^z)_{12}$	1	1	2	1	1
30.3	$O/C_2^{xy}/C_1\ (O,C_2^{xy})_{12}$	31.3	$T_d/C_s/C_1\ (O,C_2^{xy})_{12}$	1		1	1*	2*
30.4	$O/C_3/C_1\ (O,C_3)_8$	31.4	$T_d/C_3/C_1\ (O,C_3)_8$	1	1		1*	1
30.5	$O/D_2^{(z,xy,\bar{x}y)}/C_1\ (O,D_2^{(z,xy,\bar{x}y)})_6$	31.5	$T_d/C_{2v}/C_1\ (O,D_2^{(z,xy,\bar{x}y)})_6$	1		1		1*
30.6	$O/C_4/C_1\ (O,C_4)_6$	31.6	$T_d/S_4/C_1\ (O,C_4)_6$	1		1	1*	
30.7	$O/D_3/C_1\ (O,D_3)_4$	31.7	$T_d/C_{3v}/C_1\ (O,D_3)_4$	1				1*
30.8	$O/D_2^{(z,x,y)}\ (D_3)_6$	31.8	$T_d/D_2\ (D_3)_6$	1	1	2*		
30.9	$O/D_4/D_2\ (D_3,C_2)_3$	31.9	$T_d/D_{2d}/D_2\ (D_3,C_2)_3$	1		1*		
30.10	$O/T\ (C_2)_2$	31.10	$T_d/T\ (C_2)_2$	1	1*			
30.11	$O/O\ (C_1)_1$	31.11	$T_d/T_d\ (C_1)_1$	1*				

	O_h-m3m	$^s\Gamma_1^+$	Γ_2^+	$^s\Gamma_3^+$	Γ_4^+	$^s\Gamma_5^+$	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-
32.1	$O_h/C_1\ (O_h)_{48}$	1	1	2	3	3	1	1	2	3*	3*
32.2	$O_h/C_2^z/C_1\ (O_h,C_2^z)_{24}$	1	1	2	1	1	1	1	2	1	1
32.3	$O_h/C_s^z/C_1\ (O_h,C_2^z)_{24}$	1	1	2	1	1				2*	2*
32.4	$O_h/C_2^{xy}/C_1\ (O_h,C_2^{xy})_{24}$	1		1	1	2	1		1	1	2*
32.5	$O_h/C_s^{xy}/C_1\ (O_h,C_2^{xy})_{24}$	1		1	1	2		1	1	2*	1
32.6	$O_h/C_3/C_1\ (O_h,C_3)_{16}$	1	1		1	1	1	1		1	1
32.7	$O_h/C_4/C_1\ (O_h,C_4)_{12}$	1		1	1		1		1	1	
32.8	$O_h/S_4/C_1\ (O_h,C_4)_{12}$	1		1	1			1	1		1
32.9	$O_h/C_{2v}^{(z,x,y)}/C_1\ (O_h,C_{2v}^{(z,x,y)})_{12}$	1	1	2						1	1
32.10	$O_h/D_2^{(z,xy,\bar{x}y)}/C_1\ (O_h,D_2^{(z,xy,\bar{x}y)})_{12}$	1		1		1	1		1		1
32.11	$O_h/C_{2v}^{(z,xy,\bar{x}y)}/C_1\ (O_h,D_2^{(z,xy,\bar{x}y)})_{12}$	1		1		1		1	1	1	
32.12	$O_h/C_{2v}^{(xy,\bar{x}y,z)}/C_1\ (O_h,C_{2v}^{(xy,\bar{x}y,z)})_{12}$	1		1		1				1*	1*
32.13	$O_h/D_3/C_1\ (O_h,D_3)_8$	1				1	1				1*
32.14	$O_h/C_{3v}/C_1\ (O_h,D_3)_8$	1				1		1		1*	
32.15	$O_h/C_{4v}/C_1\ (O_h,C_{4v})_6$	1		1						1*	
32.16	$O_h/D_{2d}^{(z,xy,\bar{x}y)}/C_1\ (O_h,C_{4v})_6$	1		1							1*
32.17	$O_h/C_i\ (O)_{24}$	1	1	2	3*	3*					
32.18	$O_h/C_{2h}^z/C_i\ (O,C_2^z)_{12}$	1	1	2	1	1					
32.19	$O_h/C_{2h}^{xy}/C_i\ (O,C_2^{xy})_{12}$	1		1	1*	2*					
32.20	$O_h/C_{3i}/C_i\ (O,C_3)_8$	1	1		1*	1					
32.21	$O_h/C_{4h}/C_i\ (O,C_4)_6$	1		1	1*						

TABLE I. (*Continued.*)

	O_h-m3m	${}^s\Gamma_1^+$	Γ_2^+	${}^s\Gamma_3^+$	Γ_4^+	${}^s\Gamma_5^+$	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-
32.22	$O_h/D_{2h}^{(z,xy,\bar{x}y)}/C_1\ (O,D_2^{(z,xy,\bar{x}y)})_6$	1		1		1*					
32.23	$O_h/D_{3d}/C_i\ (O,D_3)_4$	1				1*					
32.24	$O_h/D_2^{(z,x,y)}\ (D_6)_{12}$	1	1	2			1	1	2*		
32.25	$O_h/D_4/D_2\ (D_6,C_2^y)_6$	1		1			1		1*		
32.26	$O_h/D_{2d}^{(z,x,y)}/D_2\ (D_6,C_2^y)_6$	1		1				1	1*		
32.27	$O_h/D_{2h}^{(z,x,y)}\ (D_3)_6$	1	1	2*							
32.28	$O_h/D_{4h}/D_{2h}\ (D_3,C_2^x)_3$	1		1*							
32.29	$O_h/T\ (D_2)_4$	1	1				1	1			
32.30	$O_h/T_d\ (C_2)_2$	1						1*			
32.31	$O_h/O\ (C_2)_2$	1					1*				
32.32	$O_h/T_h\ (C_2)_2$	1	1*								
32.33	$O_h/O_h\ (C_1)_1$	1*									

$\pi_G^{H'}(g), g\in G$, of the transitive permutation representation $\Pi_G^{H'}$ of G, corresponds an $n\times n$ matrix $D_G^{H'}(g)$ defined by

$$[D_G^{H'}(g)]_{ij}=\begin{cases}1, & \text{if } g_i^{-1}gg_j\in H'\\ 0, & \text{otherwise}\end{cases} \tag{24}$$

where g_i and g_j are coset representatives in the coset decomposition given in Eq. (15). The set of all matrices $D_G^{H'}(g)$ for all $g\in G$ constitutes an n-dimensional matrix representation $D_G^{H'}$ of G. We shall call this representation the "permutation representation" of G.

From the definition, Eq. (24), it follows that $D_G^{H'}$ is an induced representation[1,2] of G. The representation $D_G^{H'}$ is induced from the identity representation $D_{H'}^1$ of the subgroup H' of G. We denote this relationship between the representation $D_G^{H'}$ of G and $D_{H'}^1$ of H' by

$$D_G^{H'}=D_{H'}^1\uparrow G\ . \tag{25}$$

One can construct, in a similar manner, the groups of matrices $D_{G/H}^{H'/H}$, for all elements g_kH of the factor group G/H, and $D_A^{A'}$, for all elements a_k of the abstract group $A\simeq G/H$:

$$[D_{G/H}^{H'/H}(g_kH)]_{ij}=\begin{cases}1, & \text{if } (g_iH)^{-1}g_kH(g_jH)\in H'/H\\ 0, & \text{otherwise}\end{cases} \tag{26}$$

$$[D_A^{A'}(a_k)]_{ij}=\begin{cases}1, & \text{if } a_i^{-1}a_ka_j\in A'\\ 0, & \text{otherwise}\ .\end{cases} \tag{27}$$

These groups of matrices are representations of the groups G/H and A, respectively. Because of the isomorphisms of Eq. (18), these representations are equivalent. We choose the isomorphism such that the matrices are identical for each g_kH and a_k mapped into each other by this isomorphism:

$$D_{G/H}^{H'/H}(g_kH)=D_A^{A'}(a_k)\ . \tag{28}$$

It was shown above that the permutation representation $D_G^{H'}$ of G is induced by the identity representation $D_{H'}^1$ of H'. Analogously, the representation $D_{G/H}^{H'/H}$ of G/H and $D_A^{A'}$ of A are induced, respectively, by the identity representations $D_{H'/H}^1$ of H'/H and $D_{A'}^1$ of A':

$$D_{G/H}^{H'/H}=D_{H'/H}^1\uparrow G/H\ ,$$
$$D_A^{A'}=D_{A'}^1\uparrow A\ . \tag{29}$$

As will be shown below, in physical applications of color groups it is of importance that the permutation representation $D_G^{H'}$, Eq. (25), in addition to being induced by the identity representation $D^1_{H'}$ of H' can also be considered an "engendered" representation.[1] The representation $D_G^{H'}$ is engendered by the representation $D_{G/H}^{H'/H}$ of the factor group G/H or, by Eq. (28), by the representation $D_A^{A'}$ of the abstract group $A \simeq G/H$.

Engendering[1] of a representation D_G of G by a representation $D_{G/H}$ of its factor group G/H is defined as follows: Let H be a normal subgroup of G. The cosets $g_i H$ of a coset decomposition of G with respect to H,

$$G = H + g_2 H + \cdots + g_m H \ , \tag{30}$$

are elements of the factor group G/H. If $D_{G/H}$ is a representation of G/H, then to every coset $g_k H$ of the factor group G/H corresponds a matrix $D_{G/H}(g_k H)$. We define a representation D_G of G as follows: All matrices $D_G(g_k h)$ for all $h \in H$ are set equal to the matrix $D_{G/H}(g_k H)$:

$$D_G(g_k h) = D_{G/H}(g_k H) \ . \tag{31}$$

The representation D_G so defined is the representation of the group G engendered by the representation $D_{G/H}$ of its factor group G/H. We shall use the symbol

$$D_G = D_{G/H} \uparrow\uparrow G \tag{32}$$

to denote that the representation D_G of G is engendered by the representation $D_{G/H}$ of its factor group G/H.

Both representations $D_{G/H}$ and $D_{G/H} \uparrow\uparrow G$ have the same dimensions. $D_G = D_{G/H} \uparrow\uparrow G$ is an irreducible representation of G if and only if $D_{G/H}$ is an irreducible representation of G/H. If the representation $D_{G/H}$ is reducible,

$$D_{G/H} = \sum_j (D_{G/H} \mid D^j_{G/H}) D^j_{G/H} \ , \tag{33}$$

then the engendered representation, Eq. (32), is also reducible:

$$D_G = \sum_j (D_G \mid D^j_G) D^j_G \ . \tag{34}$$

Each irreducible representation D^j_G in Eq. (34) is engendered by one and only one irreducible representation $D^j_{G/H}$ contained in Eq. (33). That is,

$$D^j_G = D^j_{G/H} \uparrow\uparrow G \ , \tag{35}$$

and

$$(D_G \mid D^j_G) \equiv (D_{G/H} \uparrow\uparrow G \mid D^j_{G/H} \uparrow\uparrow G) = (D_{G/H} \mid D^j_{G/H}) \ . \tag{36}$$

Two special cases of Eqs. (34) to (36) are of importance in the application of color groups to the Landau theory of phase transitions:

(a) The permutation representation $\Pi_G^{H'}$ is engendered by $\Pi_{G/H}^{H'/H} = \Pi_A^{A'}$, Eq. (19). Correspondingly, the permutation representation $D_G^{H'}$, Eqs. (22) and (24), is engendered by $D_{G/H}^{H'/H} = D_A^{A'}$, Eqs. (26) through (28):

$$D_G^{H'} = D^1_{H'} \uparrow G = D_{G/H}^{H'/H} \uparrow\uparrow G \simeq D_A^{A'} \uparrow\uparrow G \ . \tag{37}$$

(b) Each irreducible representation D^j_G contained in the nth power of $D_G = D_{G/H} \uparrow\uparrow G$ is engendered by one and only one irreducible representation $D^j_{G/H}$ contained in the nth power of $D_{G/H}$. That is, if

$$(D_G)_n = \sum_j ((D_G)_n \mid D^j_G) D^j_G \tag{38}$$

and

$$(D_{G/H})_n = \sum_j ((D_{G/H})_n \mid D^j_{G/H}) D^j_{G/H} \ , \tag{39}$$

then

$$((D_G)_n \mid D^j_G) \equiv ((D_{G/H} \uparrow\uparrow G)_n \mid D^j_{G/H} \uparrow\uparrow G) = ((D_{G/H})_n \mid D^j_{G/H}) \ . \tag{40}$$

The above is also valid for the cases of the nth symmetrized and antisymmetrized powers of a representation $D_G = D_{G/H} \uparrow\uparrow G$. That is,

$$((D_G)_{(n)} \mid D^j_G) = ((D_{G/H})_{(n)} \mid D^j_{G/H}) \ , \tag{41}$$

$$((D_G)_{[n]} \mid D^j_G) = ((D_{G/H})_{[n]} \mid D^j_{G/H}) \ . \tag{42}$$

The symbols $(D)_{(n)}$ and $(D)_{[n]}$ denote, respectively, the nth symmetrized and antisymmetrized powers of the representation D.

A well-known example of engendered representations is the $k=0$ irreducible representations $D_G^{(k=0,\nu)}$ of a space group G. We denote the normal subgroup of primitive translations of the space group G by $T = \{(1 \mid t)\}$. We write the space group G in a coset decomposition with respect to T:

$$G = T + (\hat{g}_2 \mid \tau_2) T + \cdots + (\hat{g}_m \mid \tau_m) T \ . \tag{43}$$

The coset representatives $(\hat{g}_i \mid \tau_i)$ consist of an element $\hat{g}_i$ of the point group $\hat{G}$ of the space group G, and a nonprimitive translation τ_i associated with $\hat{g}_i$. The isomorphism between the factor group G/T and the point group $\hat{G}, G/T \simeq \hat{G}$, maps each coset $(\hat{g}_i \mid \tau_i)T$ onto an element $\hat{g}_i$ of the point group $\hat{G}$. In a $k=0$ irreducible representation $D_G^{(0,\nu)}$ of the space group G the matrices of all elements

$$(\hat{g}_i \mid \tau_i + t) \in (\hat{g}_i \mid \tau_i) T$$

are equal to the matrix $D_{\hat{G}}^{\nu}(\hat{g}_i) \equiv \Gamma_\nu(\hat{g}_i)$ of the irreducible representation $D_{\hat{G}}^{\nu} \equiv \Gamma_\nu$ of the point group $\hat{G}$:

$$D_G^{(0,\nu)}((\hat{g}_i \mid \tau_i + t)) = \Gamma_\nu(\hat{g}_i) . \quad (44)$$

Hence, a $k=0$ irreducible representation $D_G^{(0,\nu)}$ of a space group G is engendered by an irreducible representation $D_{\hat{G}}^{\nu} \equiv \Gamma_\nu$ of the point group $\hat{G}$:

$$D_G^{(0,\nu)} = D_{\hat{G}}^{\nu} \uparrow\uparrow G \equiv \Gamma_\nu \uparrow\uparrow G . \quad (45)$$

Consequently, in many calculations, one uses the irreducible representations Γ_ν of the point group $\hat{G}$ in place of the $k=0$ irreducible representations $D_G^{(0,\nu)}$ of the space group G.

The permutation representations $D_G^{H'}$, Eq. (24), are reducible. The reduction can be carried out using the theory of characters of representations.[1–4] In Table I alongside each permutational color point group $\hat{G}/\hat{H}'/H\ (A,A')_n$ isomorphic to $\hat{G}$, we have tabulated the multiplicity $(D_{\hat{G}}^{\hat{H}'} \mid D_{\hat{G}}^{j})$ with which each irreducible representation $D_{\hat{G}}^{j}$ of $\hat{G}$ is contained in the representation $D_{\hat{G}}^{\hat{H}'}$:

$$D_{\hat{G}}^{\hat{H}'} = \sum_j (D_{\hat{G}}^{\hat{H}'} \mid D_{\hat{G}}^{j}) D_{\hat{G}}^{j} . \quad (46)$$

It follows from Eqs. (23), (34)–(37), and (45), that Table I is also applicable to all permutational color space groups $G^P \simeq G$ where H' is an equitranslational subgroup of the space group G. One needs only to omit the upper index in the Schonflies notation of the space groups G, H', and H to find the corresponding point groups $\hat{G}$, $\hat{H}'$, and $\hat{H}$. The multiplicity of a $k=0$ irreducible representation $D_G^{(0,\nu)}$ in $D_G^{H'}$ is equal to the multiplicity of the irreducible representation $D_{\hat{G}}^{\nu} \equiv \Gamma_\nu$ in $D_{\hat{G}}^{\hat{H}'}$.

$$(D_G^{H'} \mid D_G^{(0,\nu)}) = (D_{\hat{G}}^{\hat{H}'} \mid D_{\hat{G}}^{\nu} \equiv \Gamma_\nu) . \quad (47)$$

The latter multiplicities are those tabulated in Table I.

V. LANDAU THEORY OF CONTINUOUS PHASE TRANSITION

The Landau theory of continuous phase transitions[3,48,49] considers a continuous phase transition between a high-symmetry phase of a crystal of symmetry G and a low-symmetry phase of symmetry H'. The high-symmetry phase is described by a density function $\rho_0(r)$. The low-symmetry phase is described by a density function $\rho_1(r)$ which can be written as

$$\rho_1(r) = \rho_0(r) + \delta\rho(r) . \quad (48)$$

The function $\delta\rho(r)$ is called the symmetry-breaking part of the density function. The low-symmetry-phase density function is expanded as

$$\rho_1(r) = \sum_j \sum_m c_m^j \Psi_m^j(r) = \rho_0(r) + {\sum_j}' \sum_m c_m^j \Psi_m^j(r) , \quad (49)$$

where the functions $\Psi_m^j(r)$ are basis functions of irreducible representations D_G^j of the high-phase-symmetry group G. The symbol $\sum'_j$ denotes summation over all irreducible representation of G excluding the identity representations D_G^1. The coefficients c_m^j are functions of pressure p and temperature T, and are called order parameters. Given the group G of the high-symmetry phase, by minimizing the thermodynamic potential $\Phi(p,T,c_m^j)$ of the crystal with the coefficients c_m^j of Eq. (49) as variational order parameters, one can determine the density function $\rho_1(r)$ and subsequently the symmetry H' of the low-symmetry phase.

If the transition from a high-symmetry G to a low-symmetry H' is a continuous phase transition associated with a line of phase transitions in the p-T plane, then the transition is associated with a single irreducible or physically irreducible representation D_G^j of G. The symmetry-breaking part $\delta\rho(r)$ of the density function $\rho_1(r)$ then has nonzero coefficients c_m^j only for coefficients corresponding to this irreducible representation. It has been shown that the irreducible representation D_G^j must then satisfy several group-theoretical criteria.[3,5,7,49] These criteria are reformulated below using the theory of permutational color groups. This reformulation simplifies the application of these group-theoretical criteria in the analysis of continuous phase transition.

A. Landau subgroup criterion

In the Landau theory, the symmetry group H' of the low-symmetry phase is a subgroup of the high-symmetry phase. All subgroups H' of G can be found in a tabulation of all permutational color groups $G/H'/H(A,A')_n$ belonging to the family of G. A partial list of permutational color space groups is given in Refs. 38, 40, and 41. A complete list of all 279 permutational color points groups is given in Table I.

B. Subduction criterion

The subduction criterion[50] is a condition restricting the irreducible representations D_G^j which can be associated with phase transitions between phases of symmetry G and H', a subgroup of G. The groups G and H' and the irreducible representation D_G^j are related by the subduction criterion

$$D_G^j \downarrow H' = \sum_i (D_G^j \downarrow H' \mid D_{H'}^i) D_{H'}^i \ ,$$

$$\text{with } (D_G^j \downarrow H' \mid D_{H'}^1) \neq 0 \ . \qquad (50)$$

That is, the irreducible representation D_G^j of G subduced on the subgroup H' must contain the identity representation $D_{H'}^1$ of H'.

The subduction criterion is used to determine the irreducible representations D_G^j which can be associated with a phase transition between phases of given symmetries G and H'. Alternatively, given the symmetry group G and irreducible representation D_G^j associated with the phase transition, it can be used to determine symmetry groups H' which can arise in a continuous phase transition.

The number of times the identity representation $D_{H'}^1$ of H' is contained in $D_G^j \downarrow H'$ is, by the Frobenious reciprocity theorem,[1] equal to the number of times D_G^j is contained in the representation $D_{H'}^1 \uparrow G$ induced by the identity representation $D_{H'}^1$ of H':

$$(D_G^j \downarrow H' \mid D_{H'}^1) = (D_{H'}^1 \uparrow G \mid D_G^j) \ . \qquad (51)$$

As was shown above in Eq. (25), the induced representation $D_{H'}^1 \uparrow G$ is the permutation representation $D_G^{H'}$ associated with the permutational color group $G/H'/H\ (A,A')_n$. Hence,

$$(D_G^j \downarrow H' \mid D_{H'}^1) = (D_G^{H'} \mid D_G^j) \ . \qquad (52)$$

Consequently, the irreducible representation D_G^j satisfies the subduction criterion for a transition between phases of symmetry G and H' if and only if D_G^j is contained in the permutation representation $D_G^{H'}$ associated with the permutational color group $G/H'/H\ (A,A')_n$.

In Table I, we have tabulated the coefficients $(D_{\hat{G}}^{\hat{H}'} \mid D_{\hat{G}}^j)$, Eq. (52), for the representation $D_{\hat{G}}^{\hat{H}'}$ associated with all permutational color point groups $\hat{G}/\hat{H}'/\hat{H}\ (A,A')_n$. These coefficeints are applicable in applying the subduction criterion to phase transitions between phases of point-group symmetries $\hat{G}$ and $\hat{H}'$. They are also applicable in applying the subduction criterion to phase transitions between phases of space-group symmetry G and H' when H' is an equitranslational subgroup of G.

For equitranslational phase transitions between space groups G and H' the coefficients $(D_{\hat{G}}^{\hat{H}'} \mid D_{\hat{G}}^j)$ found in Table I are, using Eq. (47), set equal to the coefficients $(D_G^{H'} \mid D_G^{(0,j)})$. Using Eq. (52), they determine the $k=0$ irreducible representation $D_G^{(0,j)}$ which can be associated with an equitranslational phase transition between phases of space-group symmetry G and H'. Alternatively, given the space group G and $k=0$ irreducible representation $D_G^{(0,j)}$, the coefficients $(D_{\hat{G}}^{\hat{H}'} \mid D_{\hat{G}}^j)$ found in Table I determine possible equitranslational subgroups H'.

For example, consider a phase transition between phases of symmetry $G = O_h^7$ and its equitranslational subgroup $H' = C_{4h}^6$. We first determine all possible irreducible representations which satisfy the subduction criterion for this transition. In Table I, line 32.21, for the permutation color point group $O_h/C_{4h}/C_i\ (O,C_4)_6$ we find the nonzero coefficients $(D_{O_h}^{C_{4h}} \mid D_{O_h}^j)$, Eq. (46). The reduced form of the representation $D_{\hat{G}}^{\hat{H}'}$ is then

$$D_{O_h}^{C_{4h}} = \Gamma_1^+ \oplus \Gamma_3^+ \oplus \Gamma_4^+ \ . \qquad (53)$$

Consequently, using Eq. (47), the $k=0$ irreducible representations contained in $D_{O_h^7}^{C_{4h}^6}$ are

$$D_{O_h^7}^{(0,1+)},\ D_{O_h^7}^{(0,3+)},\ D_{O_h^7}^{(0,4+)} \ . \qquad (54)$$

From Eq. (52) it follows that the subduction criterion is satisfied only for the $k=0$ irreducible representations of $G = O_h^7$ in Eq. (54).

Now consider that we are given the group $G = O_h^7$ and the irreducible representation $D_{O_h^7}^{(0,4+)} = \Gamma_4^+ \uparrow\uparrow O_h^7$ and we wish to determine all possible subgroups H' associated with this irreducible representation such that the subduction criterion is satisfied. Using Table I, subsection 32, in the column under Γ_4^+, one finds nonzero coefficients $(\Gamma_4^+ \downarrow \hat{H}' \mid D_{\hat{H}'}^1)$ for the groups $O_h/\hat{H}'/\hat{H}\ (A,A')_n$, where $H' = C_1, C_2^z, C_2^{xy}, C_s^z, C_s^{xy}, C_3, C_4, S_4, C_i, C_{2h}^z, C_{2h}^{xy}, C_{3i}$, and C_{4h}. Consequently, the possible equitranslational transitions can be subgroups H' of O_h^7, where $\hat{H}'$ is one of the point groups given above. The corresponding equitranslational subgroups H' are[51]:

$$C_1^1, C_2^3, C_s^3 C_s^4, C_3^4, C_4^6, S_4^2, C_i^1, C_{2h}^3 C_{2h}^6, C_{3i}^2, C_{4h}^6 \ . \qquad (55)$$

However, as we shall show below, most of these groups are eliminated as possible subgroups H' by some other group-theoretical criteria.

C. Kernel-core criterion

In Sec. V B we have shown that each phase transition between phases of symmetry G and H' can be associated with a permutational color group $G/H'/H\ (A,A')_n$. The first two groups in this notation for permutational color groups were used in the subduction criterion, Sec. V B restricting the groups G and H' and irreducible representation D_G^j associated with a phase transition between phases of symmetry G and H'. We shall now show that $H=\mathrm{core}H'$, Eq. (10), the third group in the permutational color group symbol $G/H'/H\ (A,A')_n$, can be used to formulate an additional group-theoretical criterion. This criterion, called the kernel-core criterion, is an additional condition restricting the groups G and H' and irreducible representation D_G^j associated with a phase transition.

If the phase transition between phases of symmetry G and H' is associated with an irreducible representation D_G^j, then the kernel of this irreducible representation, $\ker D_G^j$, is equal to $H=\mathrm{core}H'$, the core of the group H' defined by Eq. (10):

$$\ker D_G^j = H = \mathrm{core}H' \ . \tag{56}$$

The proof of this criterion is given in Appendix A.

The kernel-core criterion, Eq. (56), is applied in the same manner as the subduction criterion. It can be used to determine the irreducible representations D_G^j which can be associated with a phase transition between phases of given symmetry G and H', or, to determine possible groups H' given the group G and irreducible representation D_G^j.

In the phase transition between $G=O_h^7$ and $H'=C_{4h}^6$, for example, the corresponding permutational color space group is $O_h^7/C_{4h}^6/C_i^1\ (O,C_4)_6$. In this case $\mathrm{core}H'=C_i^1$. Consequently by the kernel-core criterion an irreducible representation D_G^j associated with this phase transition must have $\ker D_G^j=C_i^1$. Since C_i^1 is an equitranslational subgroup of O_h^7, the irreducible representation is a $k=0$ irreducible representation $D_{O_h^7}^{(0,\nu)}$ of O_h^7 with $\ker D_{O_h^7}^{(0,\nu)}=C_i^1$. This irreducible representation is engendered, Eq. (45), by an irreducible representation Γ_ν of the point group O_h with $\ker\Gamma_\nu=C_i$. From Table II, one finds that only irreducible representations $\Gamma_\nu=\Gamma_4^+$ and Γ_5^+ are such that $\ker\Gamma_\nu=C_i$. Consequently, only the irreducible representations

$$D_{O_h^7}^{(0,4+)},\ D_{O_h^7}^{(0,5+)} \tag{57}$$

satisfy the kernel-core criterion for phase transitions between phases of symmetry O_h^7 and C_{4h}^6.

The irreducible representations associated with a phase transition between phases of symmetry O_h^7 and C_{4h}^6 which satisfy subduction criterion are given in Eq. (54); those which satisfy the kernel-core criterion in Eq. (57). It follows that only the irreducible representation $D_{O_h^7}^{(0,4+)}$ satisfies both of these criteria and is the irreducible representation associated with this phase transition.

We now apply kernel-core criterion to the second example of the preceding section, that is, to determine the possible groups H' given $G=O_h^7$ and the irreducible representation $D_{O_h^7}^{(0,4+)}$. Since the kernel of the irreducible representation $D_{O_h^7}^{(0,4+)}$ is C_i^1, by the kernel-core criterion, $C_i^1=\mathrm{core}H'=H$, and H' is an equitranslational subgroup of O_h^7. This equitranslational phase is then associated with a permutational color point group $O_h/\hat{H}'/C_i\ (A,A')$, i.e., with $\hat{G}=O_h$ and $\hat{H}=C_i$. From Table I, subsection 32, one finds such permutational color point groups with:

$$\hat{H}'=C_i,C_{2h}^z,C_{2h}^{xy},C_{3i},C_{4h} \ . \tag{58}$$

The groups H' which satisfy the kernel-core criterion for a phase transition from a phase of symmetry $G=O_h^7$ associated with the irreducible representation $D_{O_h^7}^{(0,4+)}$ are[51]:

$$C_i^1,C_{2h}^3,C_{2h}^6,C_{3i}^2,C_{4h}^6 \ . \tag{59}$$

It follows from Eqs. (55) and (59) that only those subgroups H' listed in Eq. (59) satisfy both the subduction criterion and kernel-core criterion for this phase transition.

D. Chain subduction criterion

The chain subduction criterion[5–7] is a condition restricting the subgroups H' of G which can be the symmetry group of a low-symmetry phase in a phase transition associated with an irreducible representation D_G^j from a high-symmetry phase of symmetry G: Let H_2' be a subgroup of H_1' which in turn is a subgroup of G, i.e., $H_2'\subset H_1'\subset G$. In addition, let the reduced form of the subduced representation $D_G^j\downarrow H_1'$ and $D_G^j\downarrow H_2'$ be given by

$$D_G^j\downarrow H_1'=\sum_i (D_G^j\downarrow H_1' \mid D_{H_1'}^i) D_{H_1'}^i \ , \tag{60}$$

$$D_G^j\downarrow H_2'=\sum_j (D_G^j\downarrow H_2' \mid D_{H_2'}^i) D_{H_2'}^i \ . \tag{61}$$

If

$$(D_G^j\downarrow H_2' \mid D_{H_2'}^1)=(D_G^j\downarrow H_1' \mid D_{H_1'}^1) \ , \tag{62}$$

then in the phase transition from the phase of symmetry G associated with the irreducible representation D^j_G, H'_2 is eliminated as a possible symmetry group of the low-symmetry phase. If

$$(D^j_G \downarrow H'_2 \mid D^1_{H'_2}) > (D^j_G \downarrow H'_1 \mid D^1_{H'_1}) , \tag{63}$$

then the subgroup H'_2 is not eliminated.

Using Eqs. (52), Eqs. (62) and (63) can be written, respectively, as

TABLE II. Kernels of the irreducible representations of point groups: List of the 32 point groups $\hat{G}$ and their irreducible representations Γ_ν are given in the first column and row, respectively. Symbols and enumeration of the irreducible representations are that of Ref. 63. The kernel of the irreducible representation Γ_ν of the point $\hat{G}$ is given at the intersection of the column below Γ_ν and the row alongside $\hat{G}$:

	G	Γ_1 Γ_1^+ Γ_1^-	Γ_2 Γ_2^+ Γ_2^-	Γ_3 Γ_3^+ Γ_3^-	Γ_4 Γ_4^+ Γ_4^-	Γ_5 Γ_5^+ Γ_5^-	Γ_6 Γ_6^+ Γ_6^-
1	C_1	C_1					
2	C_i	C_i					
		C_i					
3	C_2	C_2	C_1				
4	C_s	C_s	C_1				
5	C_{2h}	C_{2h}	C_i				
		C_2	C_s				
6	D_2	D_2	$C_2^{(y)}$	$C_2^{(z)}$	$C_2^{(x)}$		
7	C_{2v}	C_{2v}	$C_s^{(y)}$	$C_s^{(z)}$	$C_s^{(x)}$		
8	D_{2h}	D_{2h}	$C_{2h}^{(y)}$	$C_{2h}^{(z)}$	$C_{2h}^{(x)}$		
		D_2	$C_{2v}^{(y)}$	$C_{2v}^{(z)}$	$C_{2v}^{(x)}$		
9	C_4	C_4	C_2	C_1	C_1		
10	S_4	S_4	C_2	C_1	C_1		
11	C_{4h}	C_{4h}	C_{2h}	C_i	C_i		
		C_4	S_4	C_s	C_s		
12	D_4	D_4	C_4	$D_2^{(x,y,z)}$	$D_2^{(xy,\bar{x}y,z)}$	C_1	
13	C_{4v}	C_{4v}	C_4	$C_{2v}^{(x,y,z)}$	$C_{2v}^{(xy,\bar{x}y,z)}$	C_1	
14	D_{2d}	D_{2d}	S_4	D_2	C_{2v}	C_1	
15	D_{4h}	D_{4h}	C_{4h}	$D_{2h}^{(x,y,z)}$	$D_{2h}^{(xy,\bar{x}y,z)}$	C_i	
		D_4	C_{4v}	$D_{2d}^{(x,y,z)}$	$D_{2d}^{(xy,\bar{x}y,z)}$	$C_s^{(z)}$	
16	C_3	C_3	C_1	C_1			
17	C_{3i}	C_{3i}	C_i	C_i			
		C_3	C_1	C_1			
18	D_3	D_3	C_3	C_1			
19	C_{3v}	C_{3v}	C_3	C_1			
20	D_{3d}	D_{3d}	C_{3i}	C_i			
		D_3	C_{3v}	C_1			
21	C_6	C_6	C_2	C_2	C_3	C_1	C_1
22	C_{3h}	C_{3h}	C_s	C_s	C_3	C_1	C_1
23	C_{6h}	C_{6h}	C_{2h}	C_{2h}	C_{3i}	C_i	C_i
		C_6	C_2	C_2	C_{3h}	C_s	C_s
24	D_6	D_6	C_6	$D_3^{(y,y',y'')}$	$D_3^{(x,x',x'')}$	C_1	$C_2^{(z)}$
25	C_{6v}	C_{6v}	C_6	$C_{3v}^{(y,y',y')}$	$C_{3v}^{(x,x',x'')}$	C_1	$C_2^{(z)}$
26	D_{3h}	D_{3h}	C_{3h}	D_3	C_{3v}	C_1	$C_s^{(z)}$
27	D_{6h}	D_{6h}	C_{6h}	$D_{3d}^{(y,y',y'')}$	$D_{3d}^{(x,x',x'')}$	C_i	$C_{2h}^{(z)}$
		D_6	C_{6v}	$D_{3h}^{(y,y',y'')}$	$D_{3h}^{(x,x',x'')}$	$C_s^{(z)}$	$C_2^{(z)}$
28	T	T	D_2	D_2	C_1		
29	T_h	T_h	D_{2h}	D_{2h}	C_i		
		T	D_2	D_2	C_1		
30	O	O	T	$D_2^{(x,y,z)}$	C_1	C_1	
31	T_d	T_d	T	$D_2^{(x,y,z)}$	C_1	C_1	
32	O_h	O_h	T_h	$D_{2h}^{(x,y,z)}$	C_i	C_i	
		O	T_d	$D_2^{(x,y,z)}$	C_1	C_1	

$$(D_G^{H_2'} \mid D_G^j) = (D_G^{H_1'} \mid D_G^j)\ , \tag{64}$$

$$(D_G^{H_2'} \mid D_G^j) > (D_G^{H_1'} \mid D_G^j)\ . \tag{65}$$

$D_G^{H'}$ is the permutation representation, Eq. (24), associated with the permutational color group $G/H'/H\ (A,A')_n$. For equitranslational phase transitions, using Eqs. (47), Eqs. (64) and (65) become

$$(D_{\hat{G}}^{\hat{H}_2'} \mid D_{\hat{G}}^j) = (D_{\hat{G}}^{\hat{H}_1'} \mid D_{\hat{G}}^j)\ , \tag{66}$$

$$(D_{\hat{G}}^{\hat{H}_2'} \mid D_{\hat{G}}^j) > (D_{\hat{G}}^{\hat{H}_1'} \mid D_{\hat{G}}^j)\ , \tag{67}$$

where $D_{\hat{G}}^{\hat{H}'}$ is the permutation representation associated with the permutational color point group $\hat{G}/\hat{H}'/\hat{H}\ (A,A')_n$. The values of all coefficients in Eqs. (66) and (67) are those tabulated in Table I.

We have applied the chain-subduction criterion to determine all equitranslational phase transitions. For a given irreducible representation

$$D_G^{(0,\nu)} = G_{\hat{G}}^{\nu} \uparrow\uparrow G \equiv \Gamma_\nu \uparrow\uparrow G$$

of a space group G, the equitranslational subgroups H' of G which satisfy the chain subduction criterion, Eqs. (62) and (63), have been determined using Eqs. (66) and (67) and can be found in Table I: If the coefficient

$$(D_{\hat{G}}^{H'} \mid \Gamma_\nu) \equiv (D_G^{H'} \mid D_G^{(0,\nu)})$$

at the intersection of the Γ_νth column and the row alongside the permutational color point group $\hat{G}/\hat{H}'/\hat{H}\ (A,A')_n$ is marked with an asterisk, then (a) $\hat{H}'$ is a subgroup of $\hat{G}$ which satisfies the chain subduction criterion for the irreducible representation Γ_ν, and (b) H' is an equitranslational subgroup of G which satisfies the chain subduction criterion for the $k=0$ irreducible representation $D_G^{(0,\nu)}$.

Those subgroups $\hat{H}'$ of point groups $\hat{G}$ which satisfy the chain subduction criterion for some irreducible representation Γ_ν, coincide with the possible low-symmetry point groups tabulated by Janovec, Dvorak, and Petzelt.[52] Those equitranslational subgroups H' of space groups G which satisfy the chain subduction criterion for some irreducible representation $D_G^{(0,\nu)}$ coincide with the *equitranslational epikernels* derived by Asher.[53]

As an example, we shall determine the equitranslational subgroups H' of $G=O_h^7$ which satisfy the chain subduction criterion for the $k=0$ irreducible representation

$$D_{O_h^7}^{(0,4+)} = \Gamma_4^+ \uparrow\uparrow O_h^7\ .$$

In Table I, subsection 32, in the column under Γ_4^+, one finds coefficients with an asterisk in rows alongside permutational color point groups with H':

$$C_i, C_{2h}^{xy}, C_{3i}, C_{4h}\ . \tag{68}$$

Consequently, the equitranslational subgroups H' of O_h^7 which satisfy the chain subduction criterion for the irreducible representation $D_{O_h^7}^{(0,4+)}$ are[51]

$$C_i^1, C_{2h}^3, C_{3i}^2, C_{4h}^6\ . \tag{69}$$

These groups are a subset of those which satisfied the kernel-core criterion, Eq. (59), and the subduction criterion, Eq. (55).

E. Tensor field criterion

A phase transition in a crystal is a result of a change in some physical property of the crystal. We describe the physical property by a q-component tensor function $\mathcal{T}(r)$, here called a tensor field. The components of the tensor field are $\mathcal{T}_{i\alpha} = \mathcal{T}(r_i)_\alpha$, $\alpha = 1,2,\ldots,q$, for all atomic positions r_i. The components of the tensor field transform under elements of the space group G of the crystal according to the in general reducible representation[48]:

$$D_G^{\mathrm{TF}} = D_G^T \times D_G^{\mathrm{perm}}\ . \tag{70}$$

We shall refer to the representation D_G^{TF} as the tensor field representation. The components $\mathcal{T}_{i\alpha}$, for fixed i and $\alpha=1,2,\ldots,q$, transform according to the q-dimensional tensor representation D_G^T. The permutation representation D_G^{perm} describes the permutations of the atomic positions of the crystal under elements of the space group G.

The tensor field criterion is a condition which restricts the irreducible representations which can be associated with a phase transition from a high-phase-symmetry G of a given crystal[7,50]: An irreducible representation D_G^j associated with a phase transition from a given crystal of symmetry G and due to a change in a physical property described by a tensor field $\mathcal{T}(r)$ with tensor representation D_G^T, must be contained in the tensor field representation D_G^{TF}, Eq. (70). That is,

$$D_G^{\mathrm{TF}} = \sum_i (D_G^{\mathrm{TF}} \mid D_G^i) D_G^i, \quad \text{with } (D_G^{\mathrm{TF}} \mid D_G^j) \neq 0\ . \tag{71}$$

Because the tensor representation D_G^T describes only the rotational properties of the components of the tensor, it contains only $k=0$ irreducible representation $D_G^{(0,\nu)}$ of the space group G. From Eq.

(70) it follows that the k dependence of the irreducible representation D_G^j contained in the tensor field representation D_G^{TF}, Eq. (71), is the same as the k dependence of the irreducible representations contained in the permutation representation D_G^{perm}.

To determine the irreducible representations contained in the permutation representation D_G^{perm}, it is advantageous to partition the crystal of space-group symmetry G into *simple crystals*.[12] Each simple crystal consists of all atoms whose atomic positions can be obtained by applying all elements of the space group G to any one atomic position r. The simple crystal is said to be generated by G from r. The elements of G permute atoms of each simple crystal among themselves. Consequently, the permutation representation of the atomic positions of a crystal is the direct sum of the permutation representations of the constituent simple crystals.

For a simple crystal generated by G from r_1, the permutation is given by

$$D_G^{\mathrm{perm}}=D_G^{S(r_1)}=D_{S(r_1)}^1\uparrow G\ , \tag{72}$$

where $S(r_1)$ is the subgroup of all elements g of G such that $gr_1=r_1$. The group $S(r_1)$ is called the site subgroup of the space group G at r_1.[54] Consequently, the tensor field representation, Eq. (70), for a simple crystal generated by G from r_1 can be written as

$$D_G^{\mathrm{TF}}=D_G^T\times D_G^{S(r_1)}\ . \tag{73}$$

In the case of equitranslational phase transitions, the irreducible representation D_G^j associated with the phase transition is a $k=0$ irreducible representation $D_G^{(0,\nu)}$, Eq. (45), of the space group G. The irreducible representation D_G^j must then be one of the $k=0$ irreducible representations contained in the tensor field representation D_G^{TF}. The number $(D_G^{\mathrm{TF}}\,|\,D_G^{(0,\nu)})$ of times $D_G^{(0,\nu)}$ is contained in the tensor field representation, is, by Eq. (36), equal to the number $(D_{\hat G}^{\mathrm{TF}}\,|\,D_{\hat G}^{\nu})$ of times the irreducible representation $D_{\hat G}^{\nu}$ of the point group $\hat G$ is contained in

$$D_{\hat G}^{\mathrm{TF}}=D_{\hat G}^T\times D_{\hat G}^{\hat S}(r_1)\ . \tag{74}$$

$\hat S(r_1)$ is the site point group of r_1.

As an example, consider equitranslational magnetic phase transitions in a crystal with the garnet structure. The space group $G=O_h^{10}$ and the tensor representation D_G^T is the axial vector representation Γ_4^+. The atoms occupy the $6(a)$, $24(c)$, and $24(d)$ positions[55] with the respective site point groups $\hat S(r_1)=C_{3i}$, $\hat S(r_c)=D_2^{(z,xy,\bar{x}y)}$, and $\hat S(r_d)=S_4$. Hence, there are three simple crystals. The irreducible representations of the point group O_h contained in the representation $D_{\hat G}^{\hat S(r)}$, Eq. (74), for these three simple crystals are found in Table I, subsection 32, lines 32.20, 32.10, and 32.8:

$$\begin{aligned}
D_{O_h}^{C_{3i}}&=\Gamma_1^+\oplus\Gamma_2^+\oplus\Gamma_4^+\oplus\Gamma_5^+\ ,\\
D_{O_h}^{D_2(z,xy,\bar{x}y)}&=\Gamma_1^+\oplus\Gamma_3^+\oplus\Gamma_5^+\oplus\Gamma_1^-\oplus\Gamma_3^-\oplus\Gamma_5^-\ ,\\
D_{O_h}^{S_4}&=\Gamma_1^+\oplus\Gamma_3^+\oplus\Gamma_4^+\oplus\Gamma_2^-\oplus\Gamma_3^-\oplus\Gamma_5^-\ .
\end{aligned} \tag{75}$$

From Eq. (74), the irreducible representation contained in the tensor field representation D_G^{TF} are, for the three simple crystals,

$$\begin{aligned}
D_{O_h}^{\mathrm{TF}}(a)&=\Gamma_1^+\oplus\Gamma_2^+\oplus2\Gamma_3^+\oplus3\Gamma_4^+\oplus3\Gamma_5^+\ ,\\
D_{0_h}^{\mathrm{TF}}(c)&=\Gamma_2^+\oplus\Gamma_3^+\oplus3\Gamma_4^+\oplus2\Gamma_5^+\oplus\Gamma_2^-\\
&\quad\oplus\Gamma_3^-\oplus3\Gamma_4^-\oplus2\Gamma_5^-\ ,\\
D_{O_h}^{\mathrm{TF}}(d)&=\Gamma_1^+\oplus\Gamma_3^+\oplus3\Gamma_4^+\oplus2\Gamma_5^+\oplus\Gamma_2^-\\
&\quad\oplus\Gamma_3^-\oplus2\Gamma_4^-\oplus3\Gamma_5^-\ .
\end{aligned} \tag{76}$$

It follows that irreducible representations $D_{O_h^{10}}^{(0,\nu)}\equiv\Gamma_\nu$ listed in Eq. (76) satisfy the tensor field criterion for equitranslational magnetic phase transitions on the corresponding simple crystals.

Tables of the irreducible representations contained in D_G^{TF}, Eq. (74), for all crystallographic point groups $\hat G$ and subgroups $\hat S(r)$, in the case of the axial vector tensor representation, have been given by Kovalev.[56] Berenson, Kotzev, and Litvin[57] have tabulated the irreducible representations in the cases of the axial and polar vector representations, the symmetrized square of the polar vector representation, and the product of the axial and polar vector representations.

F. Landau stability criterion

The Landau stability criterion is a condition restricting the irreducible representations which can be associated with a continuous phase transiton[3]: The symmetrized cube of an irreducible representation D_G^j associated with a continuous phase transition from a high-symmetry phase of symmetry G must not contain the identity representation D_G^1 of G,

$$(D_G^j)_{(3)}=\sum_i((D_G^j)_{(3)}\,|\,D_G^i)D_G^i,\qquad \text{with } ((D_G^j)_{(3)}\,|\,D_G^1)=0\ . \tag{77}$$

An irreducible representation D_G^j which satisfies this condition is called a "Landau-active representation."

The theory of permutational color groups allows one to determine the Landau-active representations of a large class of groups simultaneously: Let $K=\ker D_G^j$ be the kernel of the irreducible representation D_G^j, and G/K the factor group of G with respect to K. Then D_G^j is engendered by a faithful irreducible representations $D_{G/K}^j$ of the factor group G/K,

$$D_G^j = D_{G/K}^j \uparrow\uparrow G \; . \tag{78}$$

According to Eq. (40),

$$((D_G^j)_{(3)} \mid D_G^1) = ((D_{G/K}^j)_{(3)} \mid D_{G/K}^1) \; . \tag{79}$$

Consequently, the irreducible representation D_G^j of G is Landau active if and only if it is engendered, Eq. (78), by a Landau-active faithful irreducible representation $D_{G/K}^j$ of the factor group G/K where $K=\ker D_G^j$.

Equation (79) allows one to simultaneously determine whether or not all irreducible representations of groups G engendered by the same faithful irreducible representation $D_{G/K}^j$ of isomorphic factor groups G/K are Landau active. For example, the kernel of the one-dimensional real alternating representation of all groups G is a subgroup K of index two. This alternating representation is engendered by the alternating representation $D_{G/K}^j$ of the factor group $G/K \simeq C_2$. Since the alternating representation of C_2 is Landau active, the one-dimensional real alternating representation of all groups G is Landau active. This is the well-known subgroup of index two theorem.[3]

In the case of $k=0$ irreducible representations $D_G^j = D_G^{(0,\nu)}$ of a space group G, since the subgroup of primitive translations is contained in $K=\ker D_G^j$, all factor groups G/K are isomorphic to some crystallographic point group:

$$D_G^{(0,\nu)} = D_{G/K}^{\nu} \uparrow\uparrow G \; . \tag{80}$$

The irreducible representation $D_{G/K}^{\nu}$ is a faithful irreducible representation of the point group G/K. Consequently, to determine which irreducible representations $D_G^{(0,\nu)}$, satisfy the Landau stability criterion, it is sufficient to determine which faithful irreducible representations of the crystallographic point groups satisfy this condition.

There are only 12 factor groups G/K with a total of 14 physically irreducible[48] representations. Of these, only eight factor groups have at least one Landau-active faithful physically irreducible representation.[58] These factor groups and their Landau-active faithful physically irreducible representations are listed in Table III. Only these irreducible representations can engender Landau-active $k=0$ irreducible representations $D_G^{(0,\nu)}$ of a space group G.

We have determined all Landau-active $k=0$ irreducible representations using Tables II and III and Eq. (80). Each irreducible representation $D_G^{(0,\nu)}$ is engendered by, Eq. (45), an irreducible representation Γ_ν of each point group $\hat{G}$. Those irreducible representations Γ_ν listed in Table I with a superscript "s", i.e., as ${}^s\Gamma_\nu$, are *not* Landau active and do not satisfy the Landau stability criterion. Those irreducible representations listed without the superscript s *are* Landau active.

For example, for $\hat{G}=O_h$, from Table I, subsection 32, all irreducible representations Γ_ν except Γ_1^+, Γ_3^+, and Γ_5^+, satisfy the Landau stability criterion. Consequently, not all irreducible representations $D_{O_h^{10}}^{(0,\nu)}$ that are engendered by irreducible representations Γ_ν of O_h which satisfy the tensor field criterion for equitranslational magnetic phase transitions in garnet, Eq. (76), are Landau active. The irreducible representations $D_{O_h^{10}}^{(0,1+)}$, $D_{O_h^{10}}^{(0,3+)}$, and $D_{O_h^{10}}^{(0,5+)}$ are not Landau active.

G. Lifshitz homogeneity criterion

The Lifshitz homogeneity criterion is a condition restricting the irreducible representations which can be associated with a spatially homogeneous continuous phase transition[3,50,59]: The antisymmetrized square of an irreducible representation D_G^j associated with a continuous phase transition from a high-symmetry phase of symmetry G

TABLE III. Landau-active faithful irreducible representations of factor groups G/K isomorphic to crystallographic point groups: Physically irreducible representations are given in parenthesis. Enumeration and symbols Γ_ν for the irreducible representations are taken from Ref. 63.

G/K	C_2	C_4	C_6	D_4	D_6	T_h	O	O_h
$D_{G/K}^j$	Γ_2	(Γ_3,Γ_4)	(Γ_5,Γ_6)	Γ_5	Γ_5	Γ_4^-	Γ_4	Γ_4^-,Γ_5^-

must not contain an irreducible representation in common with the irreducible representations contained in the polar vector representation D_G^V of G: If

$$(D_G^j)_{[2]}=\sum_i ((D_G^j)_{[2]} \mid D_G^i) D_G^i \ , \tag{81}$$

then for all D_G^i such that $((D_G^j)_{[2]} \mid D_G^i) \neq 0$, we must have $(D_G^V \mid D_G^i)=0$.

The $k=0$ irreducible representation $D_G^{(0,\nu)}$ of a space group are by Eq. (45), engendered by an irreducible representation $D_{\hat{G}}^{\nu} \equiv \Gamma_\nu$ of the point group $\hat{G}$ satisfies the Lifshitz homogeneity criterion if and only if the irreducible representation Γ_ν or physically irreducible representation $(\Gamma_\nu+\Gamma_\nu^*)$ of $\hat{G}$ satisfies the criterion. In Table I, we have denoted by a superscript "h", i.e., Γ_ν^h or $(\Gamma_\nu+\Gamma_\nu^*)^h$, those irreducible and physically irreducible representations of the crystallographic point groups G which do *not* satisfy the Lifshitz homogeneity criterion.

VI. CLASSIFICATION OF PHASE TRANSITIONS

Permutational color groups can be used in a classification of all continuous phase transitions. Let G be the symmetry group of the high-symmetry phase and $\{H_i', H_2', \ldots\}$ the set of all subgroups of G. According to the subgroup criterion, the low-phase-symmetry group is in this set. A phase transition between G and H_i' is said to belong to the equivalence class $G/H'/H\ (A,A')_n$ of permutational color groups if the color group $G/H_i'/H\ (A,A')_n$ belongs to that class of color groups. That is, the phase transition is said to belong to that equivalence class if there is an element $g_i \in G$ such that $H_i'=g_i H' g_i^{-1}$.

In phase transitions from a high-symmetry phase of symmetry G associated with a single irreducible representation D_G^j, if the phase transition from G to H_i' satisfies all group-theoretical criteria for a continuous phase transition, then all phase transitions from G to conjugate subgroups of H_i' in G also satisfy all group-theoretical criteria. All phase transitions from G to conjugate subgroups H_i' in G are said to be equivalent and are considered as a single phase transition. With our definition of equivalence classes of permutational color groups (see Sec. III C), there is a one-to-one correspondence between equivalent phase transitions from G and equivalence classes of permutational color grops $G/H'/H\ (A,A')_n$.

For example, consider the phase transitions between phases of symmetry $G=O_h$ and $H'=C_{2h}$. There are nine isomorphic subgroups C_{2h} of O_h divided into two classes of conjugate subgroups of O_h:

$$C_{2h}^z=\{C_{2h}^x, C_{2h}^y, C_{2h}^z\} \ , \tag{82}$$

$$C_{2h}^{xy}=\{C_{2h}^{xy}, C_{2h}^{x\bar{y}}, C_{2h}^{xz}, C_{2h}^{x\bar{z}}, C_{2h}^{yz}, C_{2h}^{y\bar{z}}\} \ .$$

The corresponding classes of permutational color point groups are represented (see Table I,) by the following groups:

$$32.18\ O_h/C_{2h}^z/C_i\ (O,C_2^z)_{12} \ , \tag{83}$$

$$32.19\ O_h/C_{2h}^{xy}/C_i\ (O,C_2^{xy})_{12} \ .$$

All nine phase transitions between O_h and C_{2h}^i, $i=x,y,z,xy,\ldots,y\bar{z}$, are classified under the two permutational color groups in Eq. (83). These phase transitions are considered as two nonequivalent transitions. The low-symmetry phase is considered to have several equivalent "domains", three domains in the former, and six in the latter.

All phase transitions associated with the class of permutational color groups 32.19 [Eq. (83)], are associated with the irreducible representation Γ_4^+ of O_h, satisfy all group-theoretical criteria of Sec. V, and can be continuous phase transitions. Those phase transitions associated with the class of permutational color groups 32.18 and Γ_4^+ do not satisfy the chain subduction criterion and are not continuous phase transitions.

A second classification of phase transitions[20,23] based on permutational color groups uses the concept of "exomorphism" of phase transitions.[47,60] All phase transitions associated with classes of permutational color groups $G/H'/H\ (A,A')_n$ with the same permutation group $P=(A,A')_n$ are said to belong to the same type of exomorphic phase transitions. This classification follows from Eq. (37): The permutation representation $D_G^{H'}$ of all permutational color groups $G/H'/H\ (A,A')_n$ with the same permutation group $P=(A,A')_n$ are engendered by the same representation $D_A^{A'}$.

All phase transitions belonging to the same exomorphic type have similar properties.[47,60] In all phases transitions from high-symmetry phases of symmetry G belonging to the same exomorphic type, the Landau-active irreducible representations D_G^j are all engendered by the same Landau-active faithful irreducible representations D_A^j contained in $D_A^{A'}$.

For example, all phase transitions between groups G and subgroups H' of index two in G belong to a single exomorphic type, and are associated with classes of permutational color groups with

$P=(C_2)_2$. The Landau-active alternating irreducible presentations of the groups G associated with these phase transitions are all engendered by the Landau-active faithful alternating irreducible representation of C_2. All equitranslational phase transitions belong to 45 types of exomorphic phase transitions[47] corresponding to the 45 transitive groups of permutations $(A,A')_n$ given in Ref. 20, and found in Table I.

The classification of phase transitions into exomorphic types is useful in determining the properties of classes of phase transitions. Consider, for example, the Landau subgroup of index-three conjecture,[3] that there are no continuous phase transitions between phases of symmetry G and subgroups H' of index three in G. The classification of phase transitions into exomorphic types provides an additional proof[61,62] to this conjecture: All phase transitions between phases of symmetry G and subgroups H' of index three belong to two exomorphic types: $P=(D_3,C_2)_3=S_3$ and $P=(C_3)_3 \subset S_3$. Irreducible representations associated with these phase transitions are, by the subduction criterion, contained in permutation representations $D_G^{H'}$ which in turn are engendered by irreducible representations contained in $D_A^{A'}$. Since $D_{D_3}^{C_2}=\Gamma_1+\Gamma_3$ and $D_{C_3}^{C_1}=\Gamma_1+(\Gamma_2+\Gamma_3)$, and since none of these irreducible representations satisfy the Landau stability criterion, no irreducible representation in any $D_G^{H'}$ is Landau active. Consequently, there are no continuous phase transitions between phases of symmetry G and subgroups H' of index three in G.

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APPENDIX A: PROOF OF KERNEL-CORE CRITERION

Consider a phase transition between phases of symmetry G and H' associated with an irreducible representation D_G^j. The density function $\rho_1(r)$ of the low-symmetry phase, Eq. (49), is then written as

$$\rho_1(r)=\rho_0(r)+\sum_m c_m^j \Psi_m^j(r) . \quad \text{(A1)}$$

The functions $\Psi_m^j(r)$ are basis functions of the irreducible representation D_G^j. Since H' is the symmetry group of $\rho_1(r)$ and because, by definition, all elements of the kernel of D_G^j leave all basis functions $\Psi_m^j(r)$ simultaneously invariant, we have

$$\ker D_G^j \subset H' . \quad \text{(A2)}$$

That is, the kernel of the irreducible representation is a subgroup of the low-phase-symmetry group H'.

From Eq. (46), the irreducible representation D_G^j is contained in the permutation representation $D_G^{H'}$. Also from Eq. (46) it follows that the kernel of $D_G^{H'}$ is the intersection of the kernels of all irreducible representations D_G^i contained in $D_G^{H'}$:

$$\ker D_G^{H'}=\bigcap_i \ker D_G^i . \quad \text{(A3)}$$

In particular, for the irreducible representation D_G^j it follows from Eq. (A3) that

$$\ker D_G^{H'} \subseteq \ker D_G^j . \quad \text{(A4)}$$

The kernel of $D_G^{H'}$ is a subgroup of the kernel of D_G^j. Since the kernel of the permutation representation $D_G^{H'}$ is by Eq. (14) the group $H=\mathrm{core}H'$, we have from Eq. (A4) that

$$\mathrm{core}H' \subseteq \ker D_G^j . \quad \text{(A5)}$$

Combining Eqs. (A2) and (A5) gives

$$\mathrm{core}H' \subseteq \ker D_G^j \subseteq H' . \quad \text{(A6)}$$

Finally, since $\ker D_G^j$ is an invariant subgroup of G contained in H', and $\mathrm{core}H'$ is the *maximal* invariant subgroup of G contained in H', it follows that $\mathrm{core}H'=\ker D_G^j$, which proves the kernel-core criterion, Eq. (56).

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