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COLOUR GROUPS AND PHASE TRANSITIONS

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The theory of permutational colour groups and the representations associated with them are briefly discussed. These groups are then applied to the group-theoretical analysis and classification of continuous phase transitions, assuming the Landau theory.

1. Introduction

In many problems in solid state physics it is often necessary to determine relationships between the symmetry group G of a crystal and its subgroups H or factor groups F, and between the representations of these groups. This information can be found in the theory and tables of generalized crystallographical groups, known as "colour groups"[1,2]). The general theory of colour groups based on group extension theory, was proposed by Koptsik and Kotzev[3,4]) and has been the topic of some reviews[5–7]). The purpose of this paper is to demonstrate the advantages of the application of one type of colour groups, called permutational colour groups, in the group-theoretical analysis and classification of continuous phase transitions based on the Landau theory[8–10]) (see ref. 11 for more details and tables).

2. Permutational colour groups $G^P = G/H'/H(F, F')_n$

Let G be a crystallographic group and $P \subseteq S_n$ a transitive group of permutation of n objects, a subgroup of the symmetric group S_n. The permutational colour group G^P is defined[1-4,11,13]) as a subdirect product of P and G, i.e. it is a set of pairs of elements $\langle p, g\rangle$, $p \in P$, $g \in G$, which is a subgroup of the direct product group $P \times G$ with the same composition law

$$\langle p_1, g_1\rangle\langle p_2, g_2\rangle = \langle p_1p_2, g_1g_2\rangle \in G^P \subset P \times G. \tag{1}$$

We shall use only those colour groups G^P, which are isomorphic to G. In this case there is a homomorphism $\pi: G \to P$, and all $G^P \simeq G$ can be constructed[13]) by pairing of each $g_i \in G$ with its image $\pi(g_i) = p_i \in P \subsetneq S_n$. The set $\{\pi(g) \mid g \in G\} = \Pi_G$ is a transitive permutation representation of G. Each representation $\Pi_G^{H'}$ of dimension $n = [G : H']$ can be constructed[12]) as a set of permutations of the left cosets g_iH' of the coset decomposition of G with respect to its subgroup $H' \subset G$

$$\pi(g_k) = \begin{pmatrix} \dots g_iH' \dots \\ \dots g_kg_iH' \dots \end{pmatrix} \simeq \begin{pmatrix} \dots i \dots \\ \dots i_k \dots \end{pmatrix} = p_k \in P. \tag{2}$$

The kernel $\operatorname{Ker} \Pi_G^{H'}$ of the representation $\Pi_G^{H'}$ is an intersection of all those subgroups of G that are conjugated with H'. This intersection, called a core of H', is the maximal invariant subgroup H of G, contained in H'

$$H = \operatorname{Core} H' = \bigcap_{g \in G} gH'g^{-1} = \operatorname{Ker} \Pi_G^{H'} \lhd G. \tag{3}$$

The group $p \subsetneq S_n$ is isomorphic to the factor group $G/H = F$, considered as an abstract group F, and $H'/H = F'$ is a subgroup of F of index $n = [F : F'] = [G : H']$, with the property $\operatorname{Core} F' = C_1$. Hence, the transitive representation $\Pi_F^{F'}$ is a faithful representation of $F = G/H$ and is identical with the group of permutations $P \subsetneq S_n$. For these groups P the symbols $(F, F')_n$ were used by Koptsik and Kotzev[3]), where all 45 such groups, for the 32 point groups, were tabulated.

Permutational colour groups G^P, isomorphic to G, are completely described by the symbol $G/H'/H(F, F')_n$, which is a compact form of the diagram:

$$\begin{array}{ccccc} G & \supset & H' & \rhd & H = \operatorname{Core} H' \\ \varphi\downarrow & & \varphi\downarrow & & \varphi\downarrow \\ G/H & \supset & H'/H & \rhd & C_1 \\ \| & & \| & & \| \\ F & \supset & F' & \rhd & C_1 = \operatorname{Core} F', \end{array} \tag{4}$$

where $G/H = F \simeq (F, F')_n \subsetneq S_n$, $n = [F : F'] = [G : H']$.

Two colour groups are equivalent (and are considered as one group in the tables) if $G_1 = G_2$ and their subgroups H_1' and H_2' are conjugated in G. In this case $D_{G_1}^{H_1'}$ and $D_{G_2}^{H_2'}$ are equivalent.

Usually a large number of colour groups have the same permutation group

$P = (F, F')_n$, and a number of different groups G and H' have similar group–subgroup relations. This was a basis for a classification of the colour groups[2,3]) and it is precisely this similarity in subgroup relations which was later called[14]) an "exomorphism". For example, all 3-colour groups, and all subgroup relations between G and subgroups H' of index 3 belong to two classes, with $(F, F')_n$ equal to either $(D_3, C_2')_3$ or $(C_3, C_1)_3$; while all 2-colour groups correspondingly belong to $(C_2, C_1)_2$.

The transitive permutational representations $\Pi_G^{H'}$ and $\Pi_F^{F'}$ can be written in matrix form, as $n \times n$ matrix $D_G^{H'}$ and $D_F^{F'}$, where

$$D_G^{H'}(g_k)_{ij} = \begin{cases} 1, & \text{if } g_k g_j H' = g_i H', \quad \text{or } g_i^{-1} g_k g_j \in H', \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

Obviously, these matrices form the representation of G, induced[15]) by the trivial representation $D_{H'}^1$ of its subgroup $H' \subset G$; i.e. $D_G^{H'} = D_{H'}^1 \uparrow G$, and also $D_F^{F'} = D_{F'}^1 \uparrow F$. At the same time $D_G^{H'}$ is the representation of G, engendered[15]) by a representation $D_F^{F'}$ of its factor group $F = G/H$, $H = \text{Core } H'$ (often $D_F^{F'}$ is called[16]) the image of $D_G^{H'}$, i.e. $D_F^{F'} = \text{Im } D_G^{H'}$, where $F = G/H$, $H = \text{Ker } D_G^{H'} = \text{Core } H'$).

For the engendered representations we shall use the symbol "$\Uparrow$", i.e. $D_G^{H'} = D_F^{F'} \Uparrow G$, and each $D_G^i \in D_G^{H'}$ is engendered by some $D_F^i \in D_F^{F'}$, $D_G^i = D_F^i \Uparrow G$.

The list of all 279 non-equivalent permutational colour point groups $G/H'/H(F, F')_n$ and the reduction of the associated permutation group representations $D_G^{H'} = \Sigma_i (D_G^{H'} \mid D_G^i) D_G^i$ has been presented by Birman, Kotzev and Litvin[11]).

3. Application to Landau theory

The theory of permutational colour groups and corresponding tables[1,2,11]) can be applied in the Landau theory[8-10]) in two ways: in the classification of the transitions, and in the reformulation of the group-theoretical criteria.

If G is the group of the higher symmetry phase and $\{H_1', H_2', \ldots\}$ is the set of all its subgroups, in the list of groups $G/H'/H(F, F')_n$ one can find all possible groups $H' \subset G$ of the lower symmetry phase, one group at each class of conjugated subgroups. Then, for the given G and the chosen H' one can find the irreducible representation D_G^i, responsible for the transition by eliminating "forbidden" representations. First of all the "Subduction Criterion"[9]) is applied. In terms of colour groups this means: for G and $H' \subset G$ one finds $G/H'/H(F, F')_n$ and the permutational representation $D_G^{H'} = D_{H'}^1 \uparrow G = \Sigma_i (D_G^{H'} \mid D_G^i) D_G^i$. From the Frobenius Reciprocity Theorem[15]) it follows that all D^i_G, which are not contained in $D^{H'}_G$, are eliminated: $(D^i_G \downarrow H' \mid D^1_{H'}) = (D^1_{H'} \uparrow G \mid D^i_G)$. For the point groups (and for $k = 0$ representations of the space groups) these coefficients are tabulated by Birman, Kotzěv and Litvin[11]).

The next step is the "Kernel–Core Criterion": it was shown by Birman, Kotzev and Litvin[11]) that if the transition from G to H', is associated with a single irreducible representation, D^i_G, it should be Ker D^i_G = Core $H' = H$. In other words, for $G/H'/H(F, F')_m$, representations $D^i_G \in D^{H'}_G$, but with Ker $D^i_G \neq H$, are also eliminated. This criterion can be expressed in different form: Ker D^i_G = Core H' if and only if D^i_G is engendered by a faithful irreducible representation D^i_F of $F = G/H$ which is contained in $D^{F'}_F$. It follows that if the factor group $F = G/H$ has not any faithful irreducible representations D^i_F (when $F = D_2, D_{2h}, C_{4h}, D_{4h}, C_{6h}, D_{6h}$ for example), or if $D^i_F \notin D^{F'}_F$ for some $(F, F')_m$, then the transitions cannot be continuous for all G and H' in the corresponding $G/H'/H(F, F')_m$.

In a similar way the "Landau Stability Criterion", which eliminates each D^i_G, containing D^1_G in its symmetrized cube, should be applied. The representation D^i_G is called "Landau-active", if and only if $D^1_G \notin [D^i_G]^3$, i.e. $([D^i_G]^3 \mid D^1_G) = 0$.

But, if $D^i_G = D^i_F \Uparrow G$, then $([D^i_G]^3 \mid D^1_G) = ([D^i_F]^3 \mid D^1_F)$, where, in addition, D^i_F should be a faithful irreducible representation. The faithful irreducible representations of $F = C_3, D_3, T$, and Γ_5 of O are not Landau-active, and all transitions $G \rightarrow H'$ with G/Core $H' = C_3, D_3, T$, cannot be continuous. (This is an additional proof of the "Landau Index-3 Subgroup Theorem": all 3-colour groups, $[G:H'] = 3$, are of the type $(C_3, C_1)_3 = C_3$ and $(D_3, C_2)_3 = D_3$.)

The application of the "Chain Subduction Criterion" in the frame of colour groups is also simplified. For a fixed D^i_G it is necessary to investigate only the subgroup H' with Core H' = Ker D^i_G, i.e. a small number of colour groups $G/H'/H(F, F')_n$ with the same H and F.

The application of the permutational representations $D^{H'}_G$ in the "Tensor-Field Criterion", and many examples, together with the full tables of permutation colour groups can be found in Birman, Kotzev and Litvin[11]).

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