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The Landau theory of second-order phase transitions: $[\Gamma]^3$ and $\{\Gamma\}^2$ for crystallographic point groups

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Abstract. The symmetrized cube and the antisymmetrized square of the irreducible representations of the point groups are reduced and tabulated; these are the products which are relevant to Landau's theory of second-order phase transitions.

Many of the properties of the thirty-two point groups have been tabulated in the book by Koster *et al.* (1963, to be referred to as KDWS). These authors present character tables, basis functions, subgroup relations and Kronecker products of the point-group irreducible representations (reps). The symmetrized squares of the degenerate point-group representations were tabulated by Jahn and Teller (1937). Certain other products of the point-group irreducible representations (reps), namely the symmetrized cube and the antisymmetrized square, are of interest in the Landau theory of second-order phase transitions (Landau and Lifshitz 1958, Lyubarskii 1960, Anderson and Blount 1965, Haas 1965), and it therefore seemed to be worth while to evaluate and tabulate these products in the notation of KDWS.

The group-theoretical aspect of Landau's theory may be summarized as follows (Dimmock 1963, Ascher 1966, Birman 1966, Goldrich and Birman, to be published). If it is assumed that a crystal having a symmetry group $\mathbf{G}_0$ undergoes a second-order phase transition to a structure having the symmetry group $\mathbf{G}_1$, a group of lower order than $\mathbf{G}_0$, then (i) the symmetrized cube $[\Gamma]^3$ must not contain the totally symmetrical representation (Γ_1 or $\Gamma_1{}^+$) of $\mathbf{G}_0$, and (ii) the antisymmetrized square $\{\Gamma\}^2$ must not contain the representation of a polar vector. Γ, itself, is an irreducible representation of $\mathbf{G}_0$ that subduces onto the totally symmetrical representation (Γ_1 or $\Gamma_1{}^+$) of $\mathbf{G}_1$. We therefore consider the evaluation of these two products. The character of an element R of the group $\mathbf{G}_0$ in $[\Gamma]^3$, the symmetrized cube of the representation Γ, is given by (Lyubarskii 1960)

$$[\chi]^3(R) = \tfrac{1}{3}\chi(R^3)+\tfrac{1}{2}\chi(R^2)\chi(R)+\tfrac{1}{6}\{\chi(R)\}^3 \tag{1}$$

and in $\{\Gamma\}^2$, the antisymmetrized square, by

$$\{\chi\}^2(R) = \tfrac{1}{2}\{\chi(R)\}^2-\tfrac{1}{2}\chi(R^2). \tag{2}$$

For a non-degenerate representation of a point group equations (1) and (2) can be simplified, since in this case $X(R)$ is just equal to $D_{11}(R)$, the sole element of the one-dimensional matrix representative of R; also $D_{11}(R^2) = \{D_{11}(R)\}^2$ and $D_{11}(R^3) = \{D_{11}(R)\}^3$ from the definition of a representation. Therefore

$$\begin{aligned}[X]^3(R) &= \tfrac{1}{3}D_{11}(R^3)+\tfrac{1}{2}D_{11}(R^2)D_{11}(R)+\tfrac{1}{6}\{D_{11}(R)\}^3\\ &= \tfrac{1}{3}\{D_{11}(R)\}^3+\tfrac{1}{2}\{D_{11}(R)\}^3+\tfrac{1}{6}\{D_{11}(R)\}^3\\ &= \{\chi(R)\}^3.\end{aligned} \tag{3}$$

Similarly, one can show that

$$\{\chi\}^2(R) = 0 \tag{4}$$

for a non-degenerate representation. The expression on the right-hand side of equation (3) is simply the character of R in the triple inner Kronecker product $\Gamma\otimes\Gamma\otimes\Gamma$. We therefore conclude that if Γ is a non-degenerate representation then $\{\Gamma\}^2 = 0$, while $[\Gamma]^3$ is identical with $\Gamma\otimes\Gamma\otimes\Gamma$ and so can easily be found by a repeated use of the multiplication tables in KDWS; there is therefore no need for us to tabulate $\{\Gamma\}^2$ and $[\Gamma]^3$ for the non-degenerate representations of the point groups. If Γ is real as well as being non-degenerate, then $\Gamma\otimes\Gamma\otimes\Gamma$ is simply equal to Γ; the way in which complex representations fit into the

Landau theory requires rather special consideration anyway (Landau and Lifshitz 1958, pp. 440 and 448). Barker and Loudon (1967) assume the result of equation (3), while not stating it explicitly, and use $\Gamma\otimes\Gamma\otimes\Gamma$ rather than $[\Gamma]^3$ in discussing the Landau theory.

If Γ is a degenerate representation, the above simple results do not hold and the determination of $\{\Gamma\}^2$ and $[\Gamma]^3$ is not so straightforward. For the degenerate point-group representations $\{\Gamma\}^2$ and $[\Gamma]^3$ have been evaluated, using equations (1) and (2), and reduced; they are given in the third and fifth columns of table 1 in the notation of KDWS. The symmetrized cubes of the degenerate single-valued representations of O and T_d have been given previously by Birman (1962). In the fourth column of table 1, $\Gamma\otimes\Gamma\otimes\Gamma$ is given, which can again be determined from KDWS. For example, for Γ_4 of O or T_d table 82 of KDWS gives

$$\Gamma_4\otimes\Gamma_4\otimes\Gamma_4 = \Gamma_4\otimes(\Gamma_1+\Gamma_3+\Gamma_4+\Gamma_5) = \Gamma_1+\Gamma_2+2\Gamma_3+4\Gamma_4+3\Gamma_5. \tag{5}$$

Groups that are direct products of a point group **G** with the point group C_i are not included in table 1 since their product representations can be found from those of **G** by adding + and − signs obeying the usual rules.

Table 1

Group	Rep.	$\{\Gamma\}^2$	$\Gamma\otimes\Gamma\otimes\Gamma$	$[\Gamma]^3$
(6) D_2				
(7) C_{2v}	Γ_5	Γ_1	$4\Gamma_5$	$2\Gamma_5$
(12) D_4				
(13) C_{4v}				
(14) D_{2d}	Γ_5	Γ_2	$4\Gamma_5$	$2\Gamma_5$
	Γ_6	Γ_1	$3\Gamma_6+\Gamma_7$	$\Gamma_6+\Gamma_7$
	Γ_7	Γ_1	$\Gamma_6+3\Gamma_7$	$\Gamma_6+\Gamma_7$
(18) D_3				
(19) C_{3v}	Γ_3	Γ_2	$\Gamma_1+\Gamma_2+3\Gamma_3$	$\Gamma_1+\Gamma_2+\Gamma_3$
	Γ_4	Γ_1	$3\Gamma_4+\Gamma_5+\Gamma_6$	$\Gamma_4+\Gamma_5+\Gamma_6$
(24) D_6				
(25) C_{6v}				
(26) D_{3h}	Γ_5	Γ_2	$\Gamma_3+\Gamma_4+3\Gamma_5$	$\Gamma_3+\Gamma_4+\Gamma_5$
	Γ_6	Γ_2	$\Gamma_1+\Gamma_2+3\Gamma_6$	$\Gamma_1+\Gamma_2+\Gamma_6$
	Γ_7	Γ_1	$3\Gamma_7+\Gamma_9$	$\Gamma_7+\Gamma_9$
	Γ_8	Γ_1	$3\Gamma_8+\Gamma_9$	$\Gamma_8+\Gamma_9$
	Γ_9	Γ_1	$4\Gamma_9$	$2\Gamma_9$
(28) T	Γ_4	Γ_4	$2\Gamma_1+2\Gamma_2+2\Gamma_3+7\Gamma_4$	$\Gamma_1+3\Gamma_4$
	Γ_5	Γ_1	$2\Gamma_5+\Gamma_6+\Gamma_7$	$\Gamma_6+\Gamma_7$
	Γ_6	Γ_3	$2\Gamma_5+\Gamma_6+\Gamma_7$	$\Gamma_6+\Gamma_7$
	Γ_7	Γ_2	$2\Gamma_5+\Gamma_6+\Gamma_7$	$\Gamma_6+\Gamma_7$
(30) O				
(31) T_d	Γ_3	Γ_2	$\Gamma_1+\Gamma_2+3\Gamma_3$	$\Gamma_1+\Gamma_2+\Gamma_3$
	Γ_4	Γ_4	$\Gamma_1+\Gamma_2+2\Gamma_3+4\Gamma_4+3\Gamma_5$	$\Gamma_2+2\Gamma_4+\Gamma_5$
	Γ_5	Γ_4	$\Gamma_1+\Gamma_2+2\Gamma_3+3\Gamma_4+4\Gamma_5$	$\Gamma_1+\Gamma_4+2\Gamma_5$
	Γ_6	Γ_1	$2\Gamma_6+\Gamma_8$	Γ_8
	Γ_7	Γ_1	$2\Gamma_7+\Gamma_8$	Γ_8
	Γ_8	$\Gamma_1+\Gamma_3+\Gamma_5$	$5\Gamma_6+5\Gamma_7+11\Gamma_8$	$\Gamma_6+\Gamma_7+4\Gamma_8$

It would be a very arduous task to evaluate these products for all the representations of all the 230 space groups, and we make no attempt to do this.

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