THEOREM ABOUT THIRD ORDER INVARIANTS FOR IRREDUCIBLE REPRESENTATIONS OF SPACE GROUPS

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It is shown that there can be no more than one third order invariant for an irreducible representation of a space group.

IN the Landau[1] thermodynamic theory of phase transitions, which is based on the expansion of the thermodynamic potential in series in powers of the order parameter η, two cases can occur.

1. Because of the symmetry properties of the crystal the coefficient B(p, T) of η^3 in the expansion of the thermodynamic potential is identically zero. In this case there is one condition for the transition point—the vanishing of the coefficient A(p, T) of η^2, and consequently there is a whole line of phase transitions in the (p, T) plane.

2. B(p, T) does not vanish identically. There are then isolated points of phase transition in the (p, T) plane, determined by the conditions A(p, T) = 0, B(p, T) = 0.

The second case can occur if there is just one third order invariant, since otherwise one would obtain more than two conditions for determining two quantities (cf. formula (139.6) in [1]). In the book by Landau and Lifshitz[1] it is stated, however, that one can prove a theorem to the effect that there can be no more than one third order invariant for irreducible representations of the space groups. In terms of representation theory this means that the symmetric cube $[\tau^3]$ of the irreducible representation τ of a space group contains the identity representation no more than once (cf. [2]).

The characters of the representation $[\tau^3]$ are

$$[\chi^3](g) = {}^1\!/\!_3\chi(g^3) + {}^1\!/\!_2\chi(g^2)\chi(g) + {}^1\!/\!_6\chi^3(g). \qquad (1)$$

Here $\chi(g)$ is the character of the element g in the irreducible representation τ. The identity representation is contained in the representation $[\tau^3]$ m times, where

$$m = N^{-1}\sum_{g\in G}[{}^1\!/\!_3\chi(g^3) + {}^1\!/\!_2\chi(g^2)\chi(g) + {}^1\!/\!_6\chi^3(g)]. \qquad (2)$$

For one-dimensional representations the theorem is obviously valid. To treat irreducible representations of higher dimensionality, we transform (2):

$$m = \frac{1}{N}\sum\Big\{\frac{1}{3}\chi(g^3) + \frac{1}{2}[\chi(g^2) + \chi^2(g)]\chi(g) - \frac{1}{3}\chi^2(g)\chi(g)\Big\}$$
$$= \frac{1}{3N}\sum\chi(g^3) + \frac{2}{3N}\sum[\chi^2](g)\chi(g) - \frac{1}{3N}\sum\chi(g)\{\chi^2\}(g). \qquad (3)$$

Here $[\chi^2](g)$ and $\{\chi^2\}(g)$ are the characters of the symmetric and antisymmetric square of τ, respectively; the summation is over all elements $g\in G$.

For two-dimensional irreducible representations the first term in (3) does not exceed $^2\!/_3$, since the characters of an irreducible representation of a space group do not exceed the dimensionality of the representation; the second term is equal to $^2\!/_3 m_1$, where m_1 is the number of times that the conjugate of the particular representation is contained in $[\tau^2]$. The third term in (3) is equal to $-^1\!/_3 m_2$, where m_2 is the number of times that $\{\tau^2\}^*$ is contained in τ, if the dimensionality of $\{\tau^2\}$ is less than that of τ, or the number of times that τ^* is contained in $\{\tau^2\}$ if the dimensionality of $\{\tau^2\}$ is greater than that of τ. In the first case the third term is zero (since τ is irreducible), in the second case, or if the dimension of τ is equal to that of $\{\tau^2\}$, this term is surely not positive. For two-dimensional representations the dimension of $[\tau^2]$ is three, so that m_1 is equal to either zero or one; the dimensionality of $\{\tau^2\}$ is one. Consequently the second term in (3) does not exceed $^2\!/_3$, while the third term is zero. Thus, for two-dimensional irreducible representations, m is surely less than two, i.e., is either zero or one, QED.

Arguing in the same way as for the two-dimensional case, we find from (3) for three-dimensional irreducible representations that m is surely less than two, provided that there is at least one element of the group which does not satisfy the equation

$$\tfrac{1}{2}\chi^2(g) + \tfrac{1}{2}\chi(g^2) = 2\chi^*(g). \tag{4}$$

All the point groups (cf. [3] p. 370) having three-dimensional irreducible representations contain the class $3C_2$, whose elements have the character -1 in all the three-dimensional irreducible representations. It is easy to show that condition (4) is violated for elements of this class. Thus, for the three-dimensional irreducible representations of the point groups m again can take on only the values zero or one.

For symmorphic space groups (i.e., space groups without nonelementary translations), and also for interior points of the Brillouin zone of any of the space groups (case C) the basis functions of the irreducible representations can be written in the form (cf. [1] § 136; [2])

$$\varphi_{\mathbf{k}\alpha} = u_\alpha \psi_{\mathbf{k}}, \tag{5}$$

where the u_α are periodic functions giving some irreducible representation of the point group $G_{\mathbf{k}}$ of the wave vector, and the $\psi_{\mathbf{k}}$ are linear combinations of expressions $e^{i\mathbf{k}\cdot\mathbf{r}}$ (with equivalent values of $\mathbf{k}$). The vector $\mathbf{k}$ in (5) runs through all values in its star. For the surface of the Brillouin zone, in the case of nonsymmorphic space groups (case B), expression (5) remains valid if the u_α are the basis functions of an irreducible representation of the extended group $\tilde{G}_{\mathbf{k}}$ of the wave vector which includes, in addition to the rotations, some nonelementary translations.

In order to determine the i-th order invariants of a given irreducible representation of the space group, we should apply the projection operator P_{A_1} [2, 4, 5] to all products of i functions $\varphi_{\mathbf{k}\alpha}$. To within a normalizing factor we find:

$$\begin{aligned} P_{A_1}\varphi_{\mathbf{k}_1\alpha}\varphi_{\mathbf{k}_2\beta}\ldots\varphi_{\mathbf{k}_i\gamma} &= \sum_{g\in G} T(g)\,\varphi_{\mathbf{k}_1\alpha}\varphi_{\mathbf{k}_2\beta}\ldots\varphi_{\mathbf{k}_i\gamma} \\ &= \sum_{\mathbf{A}\in J} e^{i(\mathbf{k}_1+\mathbf{k}_2+\ldots+\mathbf{k}_i)\mathbf{A}} \sum_{g\in G/J} T(g)\,\varphi_{\mathbf{k}_1\alpha}\varphi_{\mathbf{k}_2\beta}\ldots\varphi_{\mathbf{k}_i\gamma} \\ &= \delta_{\mathbf{k}_1+\mathbf{k}_2+\ldots+\mathbf{k}_i\mathbf{b}} \sum_{g\in G_{\mathbf{k}}/J\,(G_{\mathbf{k}}/J)} T(g)\,u_\alpha u_\beta\ldots u_\gamma. \end{aligned} \tag{6}$$

Here G is the space group, J is the translation subgroup, and $\mathbf{b}$ is a reciprocal lattice vector.

From (6) it follows that in order for there to be no i-th order invariant it is sufficient that the star of the representation not contain i vectors (some possibly equal) whose sum is equivalent to zero:

$$\mathbf{k}_1 + \mathbf{k}_2 + \ldots + \mathbf{k}_i = \mathbf{b}. \tag{7}$$

We note further that if condition (7) is satisfied the projection of the functions $\varphi_{\mathbf{k}_1\alpha}\varphi_{\mathbf{k}_2\beta}\ldots\varphi_{\mathbf{k}_i\gamma}$ gives the same result as the projection of the products $u_\alpha u_\beta \ldots u_\gamma$. Thus, every i-th order invariant of the space group coincides with some i-th order invariant formed from the basis functions of the irreducible representation of the point group $G_{\mathbf{k}}$ of the wave vector (case A) or of the extended group $\tilde{G}_{\mathbf{k}}$ of the wave vector (case B). The converse is not true, in general, since the star may not contain vectors satisfying condition (7).

Thus the number of i-th order invariants of irreducible representations of the space groups surely does not exceed the number of i-th order invariants for the corresponding irreducible representation of the group $G_{\mathbf{k}}$ (case A) or of the group $\tilde{G}_{\mathbf{k}}$ (case B).

Looking through the table of weighted representations,[6] we easily verify that in case B, if the dimension of the irreducible representation of the group $\tilde{G}_{\mathbf{k}}$ is greater than two, the star of the corresponding representation of the space group does not contain any triple of vectors satisfying the condition (7) for i = 3. But for the two-dimensional irreducible representations of any group, as for all (including three-dimensional) irreducible representations of the point groups, there can be no more than one third order invariant, as shown above. Consequently, both in case A and case B, there can be no more than one third order invariant of an irreducible representation of a space group. QED.

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[1] L. D. Landau and E. M. Lifshitz, "Statisticheskaya fizika" (Statistical Physics), Nauka, 1964.

[2] G. Ya. Lyubarskiĭ, Teoriya Grupp i ee primenenie v fizike (The Application of Group Theory in Physics), Gostekhizdat, 1958, transl. Pergamon, 1960.

[3] L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, 1963, transl. Pergamon, 1965.

[4] V. Heine, Group Theory in Quantum Mechanics, Pergamon, 1960.

[5] M. A. Melvin, Revs. Modern Phys. 28, 18 (1956).

[6] O. V. Kovalev, Neprivodimye predstavleniya prostranstvennykh grupp (Irreducible Representations of the Space Groups), AN UkrSSR, 1961; transl. Gordon-Breach, N. Y., 1965.

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