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LETTER TO THE EDITOR

Representation generating theorems and interaction of improper quantities with order parameter

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Abstract. It is known that a faithful representation of a finite group generates all its irreducible representations. A question about the validity of a more general theorem is raised and its role in the theory of phase transitions discussed.

1. Introduction

The possibility of phase transitions in which the order parameter (OP) is different from other actually observed onsetting physical quantities has already been suggested by Indenbom (1960a,b). So-called improper ferroelectric or ferroelastic transitions are examples of such a situation (Dvořák 1974, Levanyuk and Sannikov 1974). The onset of 'faint' (the word we use instead of 'improper') quantities can be justified either by symmetry arguments (Neumann principle) or, more physically, as a consequence of a certain (faint) coupling of these variables with the OP. We shall discuss the link between the two approaches which is provided by the representation generating theorem.

2. Symmetry approach

Let G be the symmetry group of the high-symmetry phase, α the labels of its ireps (irreducible or physically irreducible representations), and $x^{(\alpha)} = (x_{\alpha 1}, x_{\alpha 2}, \ldots, x_{\alpha d_\alpha})$ the coordinates of the d_α-times degenerate mode transforming by the matrix irep $\Gamma_{0\alpha}(G): g \to D^{(\alpha)}(g)$ and spanning d_α-dimensional $\chi_\alpha(G)$-module L_α. Further, let $F \subset G$. By $L_{\alpha 1}(F)$ we denote a subspace of L_α which is stable (each of its vectors is invariant) under F. The dimensions $s_\alpha(F) = \dim L_{\alpha 1}(F)$ are the subduction coefficients which tell us how many times $\chi_\alpha(G)$ subduces the identity irep of F. They satisfy a relation

$$\sum_\alpha s_\alpha(F) d_\alpha = [G: F] = \text{index of } F \text{ in } G.$$

A choice of bases $\{x_{\alpha i}\}$ can be made, for any given F, such that the first $s_\alpha(F)$ variables $x_{\alpha i}$ are invariant under F. All these and only these quantities are allowed by the low-symmetry F and should arise at the transition from G to F irrespective of what the OP is.

Let us consider only single-parameter transitions. If the OP belongs to the irep $\chi_\alpha(G)$, then the low-symmetry state is determined by a vector $x_s^{(\alpha)}$ of L_α and the symmetry of the state is the stabiliser of $x_s^{(\alpha)}$. Such groups are the 'epikernels' of the irep $\chi_\alpha(G)$ (Ascher 1977). The least epikernel of $\chi_\alpha(G)$ is its kernel $H_\alpha = \ker \chi_\alpha(G) \lhd G$, which is normal in G and under which the whole space L_α is stable so that $s_\alpha(H_\alpha) = d_\alpha$. Other epikernels of $\chi_\alpha(G)$ form sets of conjugate subgroups $F_i = t_i F_1 t_i^{-1}$ in G, and their stability spaces $L_{\alpha 1}(F_i)$ are accordingly $t_i L_{\alpha 1}(F_1)$ and have the same dimension $s_\alpha(F_i) = s_\alpha(F_1) < d_\alpha$. The intersection of F_i is the kernel H_α: $\bigcap_i F_i = \ker \chi_\alpha(G)$.

Faint quantities form stable subspaces $L_{\beta 1}(F)$ in spaces L_β belonging to other ireps $\chi_\beta(G)$. If the low symmetry is just H_α, the kernel of $\chi_\alpha(G)$, then its stable subspaces consist of the whole spaces L_β. To these belong all spaces L_β, the ireps of which are engendered by the ireps of the factor group $\mathscr{H}_\alpha \approx G/H_\alpha$ and no others. The matrix irep $\Gamma_{0\alpha}(G)$ is faithful as an irep of $\mathscr{H}_\alpha$, and the above relation for dimensions gives now the Burnside theorem for the factor group: $\Sigma_\beta d_\beta^2 = [G: H_\alpha] =$ order of $\mathscr{H}_\alpha$.

Thus the symmetry arguments reveal what faint quantities, forbidden in paraphase, are allowed in ferrophase. It is desirable to show that just these quantities are appropriately coupled to the OP and to find such couplings in order to substantiate our belief in their onset and to obtain a way of calculating their behaviour.

3. Representation generating theorems and the extended integrity bases

The proof of the first part of the following theorem is given in Burnside (1955, theorem IV, p 299). The second, for us more important, part can be proved in a similar way.

Theorem. A faithful representation $\chi(G)$ of a finite group G generates all its ireps in the sense that each irep $\chi_\beta(G)$ is contained: (i) in some finite power $\chi^n(G)$ or, more strongly, (ii) in some symmetrised finite power $[\chi^m(G)]$.

With respect to the irep $\chi_\alpha(G)$ of the OP, the theorem says that this irep generates all ireps $\chi_\beta(G)$ engendered by ireps $\chi_\beta(\mathscr{H}_\alpha)$ of the factor group $\mathscr{H}_\alpha \approx G/H_\alpha$. In the language of polynomials in the OP, i.e. in $x_{\alpha i}$, part (ii) says that there exists some homogeneous polynomial $\Gamma_{0\beta}(G)$-covariant $p^{(\beta)}(x^{(\alpha)}) = (p_{\beta 1}(x^{(\alpha)}), p_{\beta 2}(x^{(\alpha)}), \ldots, p_{\beta d_\beta}(x^{(\alpha)}))$ of finite degree m. Here the polynomials $p_{\beta j}(x^{(\alpha)})$ have the same transformation properties as the variables $x_{\beta j}$, are linearly independent on L_α, and are invariant under H_α. The recently developed theory of 'extended integrity bases' (EIBS) gives a method for their calculation. The EIB of polynomials in components of the OP is determined by the image Im $\Gamma_{0\alpha}(G)$ of the irep $\Gamma_{0\alpha}(G)$ or, in other words, by the matrix group of this irep. The EIBS for images of the ireps of crystal point groups are known (Patera *et al* 1978, Kopský 1975, 1979a,b).

4. Faint interactions

The groups of the Landau theory are real groups in the sense that all their ireps can be realised on real spaces. Hence they have no half-integer (second kind or complex) ireps (= ireps equivalent to their complex conjugates but not to real ones). The integer (first kind or real) ireps and pairs of complex conjugate ireps of the third kind form only one type of invariant which can always be brought to the form $r_\alpha^2 = \Sigma_{i=1}^{d_\alpha} x_{\alpha i}^2$. From this and from the generating theorem it follows that there always exists an interaction of the spontaneous OP $x_s^{(\alpha)}$ with any faint variable $x^{(\beta)}$ of the form

$$\phi_{\alpha\beta}(x^{(\beta)}, x_s^{(\alpha)}) = B_{\alpha\beta} \sum_{j=1}^{d_\beta} x_{\beta j} p_{\beta j}(x_s^{(\alpha)}).$$

We call it the 'faint' interaction; the lowest possible degree m of $p_{\beta j}$ in $x_s^{(\alpha)}$ is the index of faintness of the faint mode $x^{(\beta)}$ with respect to the OP $x^{(\alpha)}$. Here and below we use slightly modified terminology by Aizu (1973, 1974a). Taking into account the harmonic energy $A_\beta r_\beta^2$ of the faint mode, we obtain the equilibrium condition

$$-\partial\phi/\partial x_{\beta j} = -A_\beta x_{\beta j} - B_{\alpha\beta} p_{\beta j}(x_s^{(\alpha)}) = 0,$$

where ϕ = terms without $x_{\beta j} + A_\beta r_\beta^2 + \phi_{\alpha\beta}$, $-A_\beta x_{\beta j}$ is the harmonic restoring force for $x_{\beta j}$, while the second term is the force exerted on it by the spontaneous OP. It is clear that we obtain a non-zero solution for $x_{\beta j}$ only in the case when a corresponding faint interaction exists (except maybe for exceptional values of the OP). According to the generating theorem, this interaction always exists if the low symmetry is H_α, the kernel of the irep of the OP. In this case, we grant the existence of a faint interaction for all faint variables only, so that the couplings exist just for those quantities which should occur on the grounds of symmetry arguments.

In the case of epikernels we have the following situation: the OP $x_s^{(\alpha)}$ falls now in the stability space $L_{\alpha 1}(F)$. The number of non-vanishing independent components of the OP is restricted to the first $s_\alpha(F)$ variables $x_{\alpha i}$. Further, the first $s_\beta(F)$ polynomials $p_{\beta j}(x_s^{(\alpha)})$ are invariant under F, while the remaining ones are not (recall that the $p_{\beta j}$ transform in the same way as the $x_{\beta j}$). Hence these remaining polynomials vanish as long as $x_s^{(\alpha)}$ falls in $L_{\alpha 1}(F)$. Accordingly the variables $x_{\beta j}$ with the same j vanish because the corresponding faint interaction vanishes. This is in agreement with the symmetry prediction because these are just those $x_{\beta j}$ which do not belong to $L_{\beta 1}(F)$.

5. Query

Strictly speaking, some of the first $s_\beta(F)$ polynomials $p_{\beta j}$ in a given covariant $p^{(\beta)}$, or even all of them, may vanish on $L_{\alpha 1}(F)$. Inspection of EIBs for the crystal point groups shows that this frequently happens with the lowest-degree faint interactions. It also shows, however, that in all these cases there exists an interaction of higher order for any $x_{\beta j}$ belonging to $L_{\beta 1}(F)$. This has also been realised by Aizu (1974b). Here we should introduce faintness indices for components $x_{\beta j}$ in the phase of symmetry F. From what we have said so far, it follows that the faintness index is infinite (there is no coupling) for any variable which is forbidden by symmetry; it is finite for any faint variable (allowed by symmetry), and hence coupling exists if the subgroup of the low symmetry is normal in G. It is desirable to prove that it is also finite for any symmetry-allowed variable in the case of epikernels, for the violation of this rule would bring about a strange situation in which there would be no coupling justifying an onset of a symmetry-allowed quantity.

So let us finish this Letter with a proposal to investigate whether the following conjecture, formulated as a generating theorem, holds at least for real finite groups:

Conjecture. If F is an epikernel of $\chi_\alpha(G)$, then the stability space $L_{\alpha 1}(F)$ generates the stability spaces $L_{\beta 1}(F)$, in the sense that for each component $x_{\beta j} \in L_{\beta 1}(F)$ there exists a polynomial $p_{\beta j}(x^{(\alpha)})$ which transforms as $x_{\beta j}$ and does not vanish on $L_{\alpha 1}(F)$.

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