Nonmaximal Isotropy Groups and Successive Phase Transitions

Marko V. Jarić
Physics Department, Montana State University, Bozeman, Montana 59717, [(a)] *and*
Institut des Hautes Etudes Scientifiques, Bures-sur-Yvette F-91440, France
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A phenomenological Landau model which describes a simple continuous transition from a high-symmetry phase to a phase associated with a nonmaximal isotropy subgroup—hitherto conjectured impossible—is constructed. A novel feature of the model is that a single order parameter describes successive simple continuous phase transitions between three or more phases of *different* symmetries. Effects of fluctuations are considered within a renormalization-group approach.

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One of the most frequently used theories of continuous phase transitions is the phenomenological Landau theory[1] and its renormalization-group extensions.[2] Within the Landau theory a continuous transition from a high-symmetry phase (e.g., a crystal structure with a space group symmetry $\mathcal{G}_0$) to a low-symmetry phase is determined by minimizing a fourth-degree $\mathcal{G}_0$-invariant polynomial $F(\psi)$, the Landau free energy. The multicomponent order parameter ψ spans a real representation Γ of $\mathcal{G}_0$ which is, for simple continuous transitions, irreducible on the real numbers. At the equilibrium, the order parameter minimizes the free energy and its symmetry is the low symmetry.

An explicit minimization of the free energy is often a nontrivial problem and several auxiliary criteria were developed.[3,4] In particular, it is important to observe that given the representation Γ only the isotropy subgroups may be selected by the order parameter[5,6] (for given Γ a subgroup $\mathcal{G}_1$ of $\mathcal{G}_0$ is said to be an isotropy subgroup if there is a direction of the order parameter ψ which is invariant under $\mathcal{G}_1$ but not under any larger subgroup of $\mathcal{G}_0$; $\mathcal{G}_1$ is also called the stabilizer or the little group of ψ). However, only an explicit minimization can determine which particular direction and, consequently, which particular isotropy subgroup will be selected. Such explicit minimizations in a number of concrete examples led to an essentially empirical conjecture, the maximality conjecture[7]: In a simple continuous transition, a low-symmetry group is a maximal isotropy subgroup of $\mathcal{G}_0$. This conjecture was refined and extended to the Higgs mechanism of gauge field theories to state, in its most general form[8]: A fourth degree, bounded from below polynomial in n real variables $\psi_1, \psi_2, \ldots, \psi_n$ with a maximum at the origin and whose symmetry group G_0, $G_0 \leq O(n)$, is compact (finite being a special case), and irreducible on the reals, has an absolute minimum at a maximal isotropy subgroup of G_0.[9] Although never proved, the maximality conjecture has withstood numerous tests in both phase transitions and gauge field theories for almost twenty years.[8,10,11]

In the context of continuous phase transitions the maximality conjecture has several important consequences. For example, since two or more possible low symmetries would be necessarily maximal isotropy subgroups, they could not be in group-subgroup relationship. Consequently, a transition from one to another of the low-symmetry phases, e.g., in a sequence of transitions from the high-symmetry phase, would have to be a discontinuous, first-order transition. Furthermore, since subspaces of the order-parameter space associated with the maximal isotropy subgroups are typically one-dimensional, the direction picked up by the order parameter in a low-symmetry phase would typically be temperature independent.

A counterexample to the maximality conjecture was found recently.[12] It was confirmed in that counterexample that the direction of the order parameter *necessarily* varies within a low-symmetry nonmaximal phase. However, continuous transitions between low-symmetry phases, although not excluded in principle, were not possible in that example. A different counterexample to the maximality conjecture will be given in the present Letter. In this example continuous transitions between low-symmetry phases will be possible for the first time.

All possible (quartic) Landau free energies and their symmetries for a four-component irreducible order parameter have been recently classified.[13] In this classification the order parameter is written as a quaternion $\psi = (\psi_0; \vec{\psi}) = (\psi_0; \psi_1 \psi_2 \psi_3)$. The elements and the subgroups of SO(4) are labelled with use of the fact that SO(4) is the homomorphic image of the product $SU(2) \otimes SU(2)$

while SU(2) is isomorphic with the group of unimodular quaternions.[14,15] An element of SU(2) $\otimes$ SU(2) is written as an ordered pair $[l,r]$ of two unimodular quaternions. It acts on ψ to give $l\psi r^{-1}$ which corresponds to a SO(4) rotation of ψ. It can easily be seen that both $[l,r]$ and $[-l,-r]$ of SU(2)$\otimes$SU(2) correspond to the same rotation in SO(4) (we say that they have the same image).

A subgroup of SU(2)$\otimes$SU(2) can be denoted by a pair $[L/N_L, R/N_R]$, where L and R are subgroups of SU(2) while N_L and N_R are their normal subgroups such that the quotient groups L/N_L and R/N_R are isomorphic. An element of $[L/N_L, R/N_R]$ can be written as an ordered pair of unimodular quaternions $[ln_L, rn_R] = [l,r][n_L, n_R]$, where $[n_L, n_R] \in N_L \times N_R$ and l and r are coset representatives in the left coset decompositions of L and R with respect to N_L and N_R, respectively, such that the left cosets lN_L and rN_R correspond in the isomorphism between L/N_L and R/N_R. Every subgroup of SO(4) is an image of a subgroup $[L/N_L, R/N_R]$ of SU(2)$\otimes$SU(2). I will write $G = \mathrm{Im}[L/N_L, R/N_R]$, where here Im stands for the image under the homorphism SU(2)$\otimes$SU(2) $\to$ SO(4).

I will demonstrate a counterexample to the maximality conjecture by considering a breaking of the high-symmetry group $\mathcal{G}_0 = [\bar{D}_3/\bar{C}_1, \bar{O}/\bar{D}_2]$ driven by a four-component order parameter ψ which belongs to a real irreducible representation Γ of $\mathcal{G}_0$; $\mathcal{G}_0$ is represented under Γ by the matrix group $G_0 = \mathrm{Im}[\bar{D}_3/\bar{C}_1, \bar{O}/\bar{D}_2] \leq \mathrm{SO}(4)$,[13] of order 48. We use bars to indicate the inverse image (covering) under the homomorphism SU(2) $\to$ SO(3) and we use the traditional Schoenflies notation for subgroups of SO(3).[16] The associated Landau free energy is[13]

$$F(\psi) = \sum_{\alpha=0}^{4} u_\alpha I_\alpha(\psi), \tag{1}$$

where $I_0(\psi) = \|\psi\|^2 = \sum_{\alpha=0}^{3}\psi_\alpha^2$ and $I_1(\psi) = [I_0(\psi)]^2$ are the isotropic, O(4), invariants; $I_2(4) = \sum_{\alpha=0}^{3}\psi_\alpha^4$ is the so-called cubic, B_4, invariant; while $I_3(4) = \sum[\psi_i\psi_j(\psi_k^2 - \psi_0^2) - \psi_0\psi_i(\psi_j^2 - \psi_k^2)]$, with summation over cyclic permutations of $(ijk) = (123)$. A fourth-degree free energy suffices for a simple continuous transition. [If multicritical or discontinuous transitions are allowed by including higher-degree terms in $F(\psi)$, the maximality conjecture does not apply.[8]] The complete symmetry group of $F(\psi)$ is G_0 which is real and irreducible[13] fulfilling the conditions of the conjecture.[8]

To find all extrema of $F(\psi)$ we follow the method of Ref. 17. Thus, using the chain criterion[5] we first calculate all the isotropy subgroups of G_0 and dimensionalities of associated invariant subspaces (subduction frequencies). They are listed in Table I. The isotropy subgroups G_1 and G_2 are the maximal isotropy subgroups of G_0. They are isomorphic but they are not equivalent in G_0. Both G_1 and G_2 contain nonmaximal isotropy subgroups G_3 and G_4 which contain the trivial isotropy subgroup G_5.

With use of Table I it is straightforward to determine all 81 of the real and complex solutions to the equation $\partial_\psi F = 0$ and to identify the absolute minima of F. The resulting phase diagram is shown in Fig. 1. For $u_0 > 0$ the absolute minimum is at $\psi = 0$ corresponding to the high-symmetry,

TABLE I. Inequivalent isotropy subgroups G_β of $G_0 = \mathrm{Im}[\bar{D}_3/\bar{C}_1, \bar{O}/\bar{D}_2]$; their subduction frequencies $i(G_\beta)$; an order parameter $\psi(\beta)$ whose symmetry is G_β; number $\omega(\beta)$ of order parameters equivalent to $\psi(\beta)$; and total number $s(\beta)$ of associated solutions to $\partial_\psi F = 0$.

β	G_β	$i(\beta)$	$\psi(\beta)$	$\omega(\beta)$	$s(\beta)$
0	$\mathrm{Im}[\bar{D}_3/\bar{C}_1, \bar{O}/\bar{D}_2]$	0	0	1	1
1	$\mathrm{Im}[\bar{D}_3/C_1, \bar{D}_3/C_1]$	1	$(\psi_0; 0)$	8	8
2	$\mathrm{Im}[\bar{D}_3/C_1, \bar{D}_3/C_1]'$	1	$\left(0; \frac{\psi_1}{\sqrt{3}} \frac{\psi_1}{\sqrt{3}} \frac{\psi_1}{\sqrt{3}}\right)$	8	8
3	$\mathrm{Im}[\bar{C}_3/C_1, \bar{C}_3/C_1]$	2	$\left(\psi_0; \frac{\psi_1}{\sqrt{3}} \frac{\psi_1}{\sqrt{3}} \frac{\psi_1}{\sqrt{3}}\right)$	16	16
4	$\mathrm{Im}[\bar{C}_2/C_1, \bar{C}_2/C_1]$	2	$\left(0; \psi_1 \frac{\psi_2}{\sqrt{2}} \frac{\psi_2}{\sqrt{2}}\right)$	24	48
5	C_1	4	$(\psi_0; \psi_1\psi_2\psi_3)$	48	0

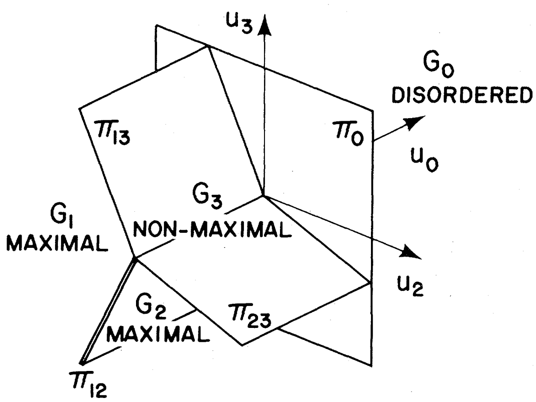

FIG. 1. Phase diagram associated with the free energy Eq. (1). Both maximal and nonmaximal ordered phases occur.

disordered phase G_0. For $u_0 < 0$ several low-symmetry, ordered phases are possible. A phase with maximal isotropy subgroup G_1 (a maximal phase) is stable for $-2u_2 > u_3 > 2u_2$ with the normalizability condition $u_2 > -u_1$ (the normalizability condition ensures that $F \to +\infty$ as $\|\psi\|^2 \to +\infty$). In this phase $\psi = (\psi_0;\,0)$ with $\psi_0^2 = -u_0/(2u_1 + 2u_2)$. Another maximal phase, G_2, is stable for $-5u_3 > 2u_2 > u_3$ where the normalizability condition is $u_2 + u_3 > -3u_1$. In this phase $\psi = \psi_1(0;111)/\sqrt{3}$ with $\psi_1^2 = -3u_0/(6u_1 + 2u_2 + 2u_3)$. These two phases are separated by a discontinuous, first-order transition along π_{12} ($u_3 = 2u_2$), where the direction of the order parameter changes abruptly. Within either of the two maximal phases only the magnitude of the order parameter changes while its direction remains fixed.

A new feature of the present model is that a phase with a nonmaximal isotropy subgroup (a nonmaximal phase) can also be stabilized. A nonmaximal phase of symmetry G_3, which is a subgroup of both G_1 and G_2, is stable for $2u_2 > \max(-u_3, -5u_3)$. The normalizability condition is quadratic: $16u_1(u_2 + u_3) + 4u_2^2 + 4u_2u_3 - 3u_3^2 > 0$. In this phase $\psi = (\sqrt{3}\,\psi_0;\,\psi_1\,\psi_1\,\psi_1)/\sqrt{3}$ and both its magnitude,

$$\|\psi\|^2 = -\frac{8u_0(u_2 + u_3)}{16u_1(u_2 + u_3) + (2u_2 + 3u_3)(2u_2 - u_3)}, \quad (2)$$

as well as its direction,

$$(\psi_1/\psi_0)^2 = \frac{6u_2 + 3u_3}{2u_2 + 5u_3}, \quad (3)$$

vary within the phase (u's are functions of temperature and other thermodynamic variables).

This example illustrates that contrary to the maximality conjecture a simple continuous phase transition between a disordered phase and an ordered nonmaximal phase is possible. Furthermore, the transitions between ordered phases G_1 and G_3 along π_{13} ($u_3 = -2u_2$) as well as between G_2 and G_3 along π_{23} ($5u_3 = -2u_2$) are simple continuous transitions. Thus, we find for the first time a possibility of describing by a single order parameter successive simple continuous transitions between three or more phases of different symmetry. Successive phase transitions are often observed, most notably in mixed perovskitetype oxides of the form $(1-x)ABO_3 + xA'B'O_3$.[18] In $(Ba_{1-x}Sr_x)TiO_3$, for example, successive transitions between cubic, tetragonal, orthorhombic, and rhombohedral phases are observed. In such cases a single (multicomponent) order parameter, phenomenological Landau model has been developed.[18] This model is, unlike the present example, capable of describing only discontinuous transitions between low-symmetry phases.

Effects of fluctuations on the phase diagram of Fig. 1 can be determined with use of a renormalization-group approach. Transitions between a disordered phase and ordered phases for all inequivalent quartic Landau free energies of a four-component order parameter were analyzed in Ref. 19 with use of the renormalization-group approach.[2] As a particular case the free energy Eq. (1) was considered and no stable fixed point was found. Therefore, the phase boundary π_0, Fig. 1, is replaced as a result of fluctuations by a first-order transition surface.

Fluctuations also affect the transitions between ordered phases. To evaluate such an effect on the transition between maximal G_1 phase and nonmaximal G_3 phase, I expand the free energy Eq. (1) around its G_1 minimum to fourth order in $\psi^{\perp}(1) = (0;\,\psi_1\psi_2\psi_3)$, the component of ψ perpendicular to $\psi(1) = (\psi_0;0)$. The quadratic term of the expansion is a bilinear form in $(\psi_1\,\psi_2\,\psi_3)$ whose eigenvalues are $\lambda_1 = u_0(2u_2 + u_3)/(2u_1 + 2u_2)$ and $\lambda_2 = \lambda_3 = u_0(4u_2 - u_3)/(4u_1 + 4u_2)$. Only λ_1 becomes critical within the domain of G_1 phase. Consequently, the expansion needs to be restricted to the λ_1 eigendirection $\psi_1(0;111)/\sqrt{3}$, giving

$$F(\psi_1) = a + \lambda_1\psi_1^2 + c\,\psi_1^4, \quad c > 0. \quad (4)$$

This free energy leads to a stable Ising-like fixed point indicating that the transition surface π_{13} remains second order sufficiently far from the intersection with the surfaces π_{23} and π_{12}. The associated criticality is Ising-like. Similarly, the transition across the surface π_{23} remains continuous and the associated criticality is Ising-like. I note, however, that transitions across π_{13} and π_{23} might become first order sufficiently near their intersection, leading to two lines of tricritical points.

Fluctuations are also expected to alter the intersections of various transition surfaces. In general, the first-order transition surface π_0 will not be smooth across its intersection with the first-order surface π_{12}. However, the cusp it will develop will have to be consistent with the 180° rule: At a point in a plane where three first-order lines meet no phase can occupy more than 180°.[20] The 180° rule, equally applicable to points where two second-order lines meet with a first-order line, is clearly satisfied at the intersection of π_{13}, π_{23}, and π_{12}. Within the Landau theory the surface π_0 is smooth across its intersections with both π_{13} and π_{23}. This feature need not be altered by a renormalization-group calculation.

In conclusion, because of the breakdown of the maximality conjecture, a minimization of a Landau free energy, or of a Higgs potential, with respect to the maximal isotropy subgroups is not sufficient. Rather, a complete minimization scheme, such as given in Ref. 17, has to be followed. The breakdown of the maximality conjecture may also shed new light on successive transitions in cases like $PbTiO_3$ where the symmetry is lowered in two successive *continuous* transitions.[21]

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[16]For example, $\overline{D}_3$ is the covering of $D_3\in$ SO(3) in SU(2); $\overline{C}_1$, a two-element group $\{1,-1\}$, is the covering of C_1 since both quaternions, 1 and -1, are mapped into the identity of SO(3). The four-fold axes of O are the coordinate axes while the threefold axis of D_3 is along the (111) direction.

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