PHYSICAL REVIEW B VOLUME 16, NUMBER 5 1 SEPTEMBER 1977

Crossover from first-order to second-order transitions in some cubic magnetic systems under pressure*

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(Received 17 March 1977)

We examine the effect of pressure on the order of phase transition in some antiferromagnetic systems in which the transition is of first order at zero pressure. By using the renormalization-group equatiðns we give a qualitative description of how the transition changes from first to second order as a uniaxial stress is applied.

The modern theory of continuous phase transitions uses the renormalization-group method[1] to describe the critical phenomena near a second-order phase-transition point. This theory was able to account properly for the effect of critical fluctuations in the values of the critical exponents in contrast to the classical Landau theory which neglects completely the fluctuations. As a further development, it has been shown recently by Brazovsky and Dzyaloshinsky[2] and Bak, Krinsky, and Mukamel[3] using the renormalization group that the Landau-theory predictions on whether a phase transition can be second-order or is necessarily a first-order transition are not always correct. The critical fluctuations can prohibit the transition from being second order. This is manifested in the renormalization-group calculation[4] in the nonexistence of stable fixed points.

There is a proof by Brézin *et al.*,[5] which states that there is always at least one stable fixed point, the isotropic fixed point, when the number of components of the order parameter is less than four. The above described situation with no stable fixed points can therefore occur only for models where the number of components is at least four. Mukamel and co-workers[3,4] have shown that many physically interesting magnetic systems are in fact described by order parameters with $n \geq 4$. For several antiferromagnetic systems, MnO and UO_2, e.g., the experiments clearly show that the transition is of first order.

It has also been observed experimentally,[6] that in some of these antiferromagnetic systems the order of the transition changes under pressure. A qualitative description of this phenomenon has been given by Bak *et al.*[7] They have pointed out that a nonisotropic stress can lift the degeneracy in the components of the order parameter, thus reducing the number of critical compoents. If the number of critical components is less than four the system can then be scaled to a stable fixed point and the transition will be second order.

The question one may ask is whether an arbitrary small pressure, which will produce a very weak tetragonal or orthorombic anisotropy, can change the nature of the transition, or if a finite distortion is required, what will determine its value. Bak *et al.*[7] answer this question in a qualitative way saying that at small pressure the components are almost degenerate and the noncritical but almost-critical components will renormalize the coupling constants of the critical components. This renormalization effect determines whether the system can have a stable fixed point or not. In this paper we want to formulate this statement in a somewhat more quantitative way and give a procedure by which this renormalization effect can be calculated. The procedure is described for the special case of UO_2 which has the dimensionality of the order parameter equal to 6 and belongs to the space group $Fm3m$ (O_h^5).[8] The analysis follows analogously for systems with different n values such as MnO ($n = 8$) and will not be given here.

The Ginzburg-Landau-Wilson Hamiltonian corresponding to the particular model with a six-component order parameter (the notation follows Mukamel and Krinsky[4]) is

$$H = \int d^dx \left(\frac{1}{2} \sum_{i=1}^{3} [r_0(\phi_i^2 + \overline{\phi}_i^2) + (\nabla\phi_i)^2 + (\nabla\overline{\phi}_i)^2] + \frac{1}{4!} g_0 \sum_{i=1}^{3} (\phi_i^4 + \overline{\phi}_i^4) + \tfrac{1}{4} g_1 \sum_{i=1}^{3} \phi_i^2\overline{\phi}_i^2 + \tfrac{1}{4} g_2 (\phi_1^2\overline{\phi}_2^2 + \phi_2^2\overline{\phi}_3^2 + \phi_3^2\overline{\phi}_1^2) \right.$$
$$\left. + \tfrac{1}{4} g_3 (\phi_1^2\overline{\phi}_3^2 + \phi_2^2\overline{\phi}_1^2 + \phi_3^2\overline{\phi}_2^2) + \tfrac{1}{4} g_4 (\phi_1^2\phi_2^2 + \phi_1^2\phi_3^2 + \phi_2^2\phi_3^2 + \overline{\phi}_1^2\overline{\phi}_2^2 + \overline{\phi}_1^2\overline{\phi}_3^2 + \overline{\phi}_2^2\overline{\phi}_3^2) \right) . \quad (1)$$

This is the Hamiltonian for the system without external stress. We know that it has no stable fixed point in the ϵ expansion to first[4] or second[9] order in ϵ, indicating that the transition should be of first order.

Let us assume that a uniaxial stress along the z axis is applied to this cubic system and it becomes tetragonal. This will split the six-dimensional irreducible representation into three two-dimensional representations, where ϕ_1 and $\overline{\phi}_2$, ϕ_2 and $\overline{\phi}_1$, and ϕ_3 and $\overline{\phi}_3$ belong to the same representation. Using the symmetry properties of the tetragonal phase and writing all the possible second- and fourth-order invariants, the Ginzburg-Landau-Wilson functional will have the form

$$H = \int d^dx \Big(\tfrac{1}{2} r_{01}(\phi_1^2 + \overline{\phi}_2^2) + \tfrac{1}{2} r_{02}(\phi_2^2 + \overline{\phi}_1^2) + \tfrac{1}{2} r_{03}(\phi_3^2 + \overline{\phi}_3^2) + \frac{1}{2} \sum_{i=1}^{3} [(\nabla\phi_i)^2 + (\nabla\overline{\phi}_i)^2] + \frac{1}{4!} g_{01}(\phi_1^4 + \overline{\phi}_2^4)$$
$$+ \frac{1}{4!} g_{02}(\phi_2^4 + \overline{\phi}_1^4) + \frac{1}{4!} g_{03}(\phi_3^4 + \overline{\phi}_3^4) + \tfrac{1}{4} g_{11}(\phi_1^2\overline{\phi}_1^2 + \phi_2^2\overline{\phi}_2^2) + \tfrac{1}{4} g_{12}\phi_3^2\overline{\phi}_3^2 + \tfrac{1}{4} g_{21}(\phi_2^2\overline{\phi}_3^2 + \phi_3^2\overline{\phi}_1^2) + \tfrac{1}{4} g_{22}\phi_1^2\overline{\phi}_2^2$$
$$+ \tfrac{1}{4} g_{31}(\phi_3^2\overline{\phi}_2^2 + \phi_1^2\overline{\phi}_3^2) + \tfrac{1}{4} g_{32}\phi_2^2\overline{\phi}_1^2 + \tfrac{1}{4} g_{41}(\phi_1^2\phi_2^2 + \overline{\phi}_1^2\overline{\phi}_2^2) + \tfrac{1}{4} g_{42}(\phi_1^2\phi_3^2 + \overline{\phi}_2^2\overline{\phi}_3^2) + \tfrac{1}{4} g_{43}(\phi_2^2\phi_3^2 + \overline{\phi}_1^2\overline{\phi}_3^2) \Big). \qquad (2)$$

The choice of the invariants is convenient, because it clearly shows how the original couplings g_i split under pressure.

The really important point here is not the splitting of the couplings, but the splitting of r_0 into r_{01}, r_{02}, and r_{03}. In the Hamiltonian (1) r_0 is a measure of the temperature, it is proportional to T. It is usually convenient to introduce r instead of r_0 by measuring the temperature relative to the critical temperature T_c, i.e., $r \sim (T - t_c)^\gamma$. Performing such a subtraction for the system under pressure, we can introduce r_1, r_2, and r_3 but now only one of them is proportional to $T - T_c$, the others remain finite at T_c. In order to be a little more specific we shall study the case when the pressure is applied in the z direction and the ferromagnetic sheets are in the (x,y) plane. In that case, the critical modes are ϕ_3 and $\overline{\phi}_3$, r_3 vanishes at T_c. The other components are not critical, r_1 and r_2 may be small at small pressure but they do not vanish. The question is how can one take into account the effect of these nearly critical components in the behavior of the system.

A convenient way to study this problem is to use the Gell-Mann-Low multiplicative renormalization in a somewhat modified form, using the physical cutoff as a scaling parameter.[10] The basic idea of that approach is that the Green's functions and vertices, when calculated with a finite-momentum cutoff Λ, obey asymptotically, near the critical temperature and for small momenta, a Gell-Mann-Low–type multiplicative renormalization relation with the cutoff as a scaling parameter. More precisely, the original problem with cutoff Λ and couplings g_i can be mapped on a problem with cutoff Λ' and couplings g_i', in such a way that the Green's functions and vertices in the two systems differ only by a multiplicative factor, independently of the momenta and temperature variable. Such relations can hold only if instead of r_1, r_2, and r_3 the renormalized masses κ_1^2, κ_2^2, and κ_3^2 are introduced by the definitions

$$G_1^{-1}(p^2, \kappa_1^2, \kappa_2^2, \kappa_3^2)\Big|_{p^2=-\kappa_1^2} = 0\,, \qquad (3)$$

$$G_2^{-1}(p^2, \kappa_1^2, \kappa_2^2, \kappa_3^2)\Big|_{p^2=-\kappa_2^2} = 0\,, \qquad (4)$$

$$G_3^{-1}(p^2, \kappa_1^2, \kappa_2^2, \kappa_3^2)\Big|_{p^2=-\kappa_3^2} = 0\,, \qquad (5)$$

where G_1, G_2, and G_3 are the Green's functions for the components ϕ_1 and $\overline{\phi}_2$, ϕ_2 and $\overline{\phi}_1$, and ϕ_3 and $\overline{\phi}_3$, respectively. One of the renormalized masses say κ_3, vanishes at T_c, the others remain finite. Introducing the dimensionless Green's functions $d_1 = G_1/G_1^{(0)}$, $d_2 = G_2/G_2^{(0)}$ and $d_3 = G_3/G_3^{(0)}$ and the dimensionless vertices $\tilde{\Gamma}_i$ corresponding to the twelve couplings, the following scaling equations hold

$$d_j\left(\frac{p^2}{\Lambda'^2}, \frac{\kappa_1^2}{\Lambda'^2}, \frac{\kappa_2^2}{\Lambda'^2}, \frac{\kappa_3^2}{\Lambda'^2}, \frac{g_i'}{\Lambda'^\epsilon}\right) = z_j\left(\frac{\Lambda'^2}{\Lambda^2}, \frac{g_i}{\Lambda^3}\right) d_j\left(\frac{p^2}{\Lambda^2}, \frac{\kappa_1^2}{\Lambda^2}, \frac{\kappa_2^2}{\Lambda^2}, \frac{\kappa_3^2}{\Lambda^2}, \frac{g_i}{\Lambda^\epsilon}\right), \quad j = 1, 2, 3 \qquad (6)$$

$$\tilde{\Gamma}_{0j}\left(\frac{p_i^2}{\Lambda'^2}, \frac{\kappa_1^2}{\Lambda'^2}, \frac{\kappa_2^2}{\Lambda'^2}, \frac{\kappa_3^2}{\Lambda'^2}, \frac{g_i'}{\Lambda'^\epsilon}\right) = z_{0j}^{-1}\left(\frac{\Lambda'^2}{\Lambda^2}, \frac{g_i}{\Lambda^\epsilon}\right) \tilde{\Gamma}_{0j}\left(\frac{p_i^2}{\Lambda^2}, \frac{\kappa_1^2}{\Lambda^2}, \frac{\kappa_2^2}{\Lambda^2}, \frac{\kappa_3^3}{\Lambda^2}, \frac{g_i}{\Lambda^\epsilon}\right), \quad j = 1, 2, 3 \qquad (7)$$

$$g_{0j}' = g_{0j}\, z_{0j}\left(\frac{\Lambda'^2}{\Lambda^2}, \frac{g_i}{\Lambda^\epsilon}\right) \cdot z_j^{-2}\left(\frac{\Lambda'^2}{\Lambda^2}, \frac{g_i}{\Lambda^\epsilon}\right), \quad j = 1, 2, 3 \qquad (8)$$

$$\tilde{\Gamma}_{11}\left(\frac{p_i^2}{\Lambda'^2},\frac{\kappa_1^2}{\Lambda'^2},\frac{\kappa_2^2}{\Lambda'^2},\frac{\kappa_3^2}{\Lambda'^2},\frac{g_i'}{\Lambda'^\epsilon}\right)=z_{11}^{-1}\left(\frac{\Lambda'^2}{\Lambda^2},\frac{g_i}{\Lambda^3}\right)\tilde{\Gamma}_{11}\left(\frac{p_i^2}{\Lambda^2},\frac{\kappa_1^2}{\Lambda^2},\frac{\kappa_2^2}{\Lambda^2},\frac{\kappa_3^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right) \tag{9}$$

$$g_{11}'=g_{11}z_{11}\left(\frac{\Lambda'^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right)z_1^{-1}\left(\frac{\Lambda'^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right)z_2^{-1}\left(\frac{\Lambda'^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right), \tag{10}$$

and similar equations for the other couplings.

We performed the calculations to lowest order in ϵ in two limiting cases: (i) when κ_3^2 is much smaller than κ_1^2 and κ_2^2 very near to T_c; and (ii) when κ_1^2, κ_2^2, and κ_3^2 are not equal but are of the same order of magnitude. In both cases, we assume that κ_1 and κ_2 are still much smaller than the physical momentum cutoff Λ. Therefore, we restrict ourselves to the leading logarithmic approximation and collect the $g_i \ln(\kappa_j^2/\Lambda^2)$ and $g_i^2 \ln^2(\kappa_j^2/\Lambda^2)$ terms.

In these two cases the multiplicative factors and the invariant couplings turn out to be the same, independent of the choice of κ_j, indicating that the scaling equations (6)–(10) can be satisfied. The renormalization-group equations for the new couplings are rather lengthy and are not given here. In addition to the fixed points which were present in the cubic case, there is the tetragonal fixed point with $g_{03}^* \neq 0$ and $g_{12}^* \neq 0$ and all the other couplings are zero, and many other fixed points. None of these fixed points is stable against perturbations given by the other couplings, if one looks at the renormalization-group equations of the couplings formally.

One should remember that a fixed point can be reached when the new cutoff is scaled down to zero, and so we reach a situation where the masses κ_1 and κ_2 are much larger than the cutoff. The renormalization-group equations can be used reasonably only until the new cutoff Λ' becomes equal to the largest of the κ_j's, say κ_1. The equations then have the form

$$d_j\left(\frac{p^2}{\Lambda^2},\frac{\kappa_1^2}{\Lambda^2},\frac{\kappa_2^2}{\Lambda^2},\frac{\kappa_3^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right) = z_j^{-1}\left(\frac{\kappa_1^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right)d_j\left(\frac{p^2}{\kappa_1^2},1,\frac{\kappa_2^2}{\kappa_1^2},\frac{\kappa_3^2}{\kappa_1^2},\frac{\bar{g}_i}{\kappa_1^\epsilon}\right), \tag{11}$$

$$\tilde{\Gamma}_{0j}\left(\frac{p^2}{\Lambda^2},\frac{\kappa_1^2}{\Lambda^2},\frac{\kappa_2^2}{\Lambda^2},\frac{\kappa_3^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right) = z_{0j}\left(\frac{\kappa_1^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right)\tilde{\Gamma}_{0j}\left(\frac{p_i^2}{\kappa_1^2},1,\frac{\kappa_2^2}{\kappa_1^2},\frac{\kappa_3^2}{\kappa_1^2},\frac{\bar{g}_i}{\kappa_1^\epsilon}\right), \tag{12}$$

$$\bar{g}_{0j}=g_{0j}z_{0j}\left(\frac{\kappa_1^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right)z_j^{-2}\left(\frac{\kappa_1^2}{\Lambda^2},\frac{g_i}{\Lambda^\epsilon}\right), \tag{13}$$

and similar equations for the other couplings. The original problem is mapped on a new problem in which one of the variables is 1. Looking at the Green's functions and vertices of the new problem, the logarithmic terms, when the argument is 1, give no contribution, and one can easily convince one's self that these functions are the same as that of the model with fields ϕ_2, $\overline{\phi}_1$, ϕ_3, and $\overline{\phi}_3$ and couplings $\bar{g}_{02},\bar{g}_{03},\bar{g}_{12},\bar{g}_{21},\bar{g}_{32},\bar{g}_{43}$ only, and all the terms which are related to ϕ_1 and ϕ_2 having renormalized mass κ_1, are frozen out. This means that apart from multiplicative factors which depend on κ_1^2/Λ^2, the original six-component problem with 12 couplings is equivalent to a four-component problem with 6 couplings.

A similar renormalization procedure can now be applied to this new problem with the new couplings $\bar{g}_{02}$, $\bar{g}_{03}$, ..., and effective cutoff κ_1. The cutoff is scaled down until we reach κ_2 and again one can convince oneself that in this way, the four-component problem can be mapped into a new two-component problem, where only the components ϕ_3 and $\overline{\phi}_3$ with couplings g_{03} and g_{12} survive, now with an effective value $\tilde{g}_{03}$ and $\tilde{g}_{12}$. The above procedure gives a straightforward prescription, of how these couplings should be calculated. If $\tilde{g}_{03}$ and $\tilde{g}_{12}$ are in the domain of attraction of the stable fixed point of this two-component system $\tilde{g}_{03}^* = \frac{3}{5}\epsilon, \tilde{g}_{12}^* = \frac{1}{5}\epsilon$, then we will finally obtain a second-order transition. The requirement for this is $\tilde{g}_{12} > 0$ and $\tilde{g}_{03} - \tilde{g}_{12} > 0$.

We can now describe the effect of pressure in a simple way. For small pressure, κ_1 is too small at the critical point and the first step in the scaling when Λ' reaches κ_1 takes us way down the scaling trajectory of the couplings. Since there is no fixed point on this trajectory, g_{03} is scaled to large negative values.[11] From there the stable fixed point of the two-component system cannot be reached in the next steps. If, however, the pressure is large, we stop on the scaling trajectories of the six-component system very early, when $\bar{g}_{03}$ is still positive and finally we can get to the stable fixed point of the two-component system.

Whenever we reach the stable fixed point of the two-component tetragonal system, the critical behavior is governed by the fixed point value and the noncritical components do not influence the critical behavior. This follows automatically for the Green's function, for which the scaling equations have been shown to hold. It does not follow from these formulas, however, that other quantities like the specific heat have the usual value for the critical exponent. It has been shown[10] that the specific heat does not obey a scaling relation similar to Eqs. (6)–(10). It is, however, possible to introduce an auxiliary quantity which obeys scaling and by which the specific heat exponent can be determined. Using the same procedure for the present problem it can be shown that the specific-heat exponent for large pressure is the same as for an ordinary tetragonal system as expected.

After we completed this work, we received a paper by Domany, Mukamel, and Fisher[12] who consider systems which classically are predicted to exhibit second-order phase transitions but known to yield first-order transitions within the renormalization-group approach because the stable fixed points are not physically accessible. Their calculation differs from ours since we consider a different case, where no stable fixed points exist.

One of us (J.S.) is grateful to the Physics Department of Rutgers University for their hospitality and for financing his stay at Rutgers where most of the present work was done.

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*Supported in part by the NSF under Grant Nos. DMR72-03230-AO1 and DMR75-13350.

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