PHYSICAL REVIEW B VOLUME 8, NUMBER 9 1 NOVEMBER 1973

Critical Behavior of Anisotropic Cubic Systems

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(Received 7 May 1973)

The critical behavior in zero field above T_c of ferromagnets or ferroelectrics with a Hamiltonian of cubic symmetry is studied, to order ϵ^2, by exact renormalization-group techniques in $d = 4 - \epsilon$ dimensions with n-component spins. For $\epsilon = 1$, $n \geq 3$, a crossover from isotropic (Heisenberg) to characteristic cubic behavior occurs, with the new value $2\nu^C = 1 + [(n-1)/3n]\epsilon + [(n-1)/324n^3](17n^2 + 290n - 424)\epsilon^2 + O(\epsilon^3)$, and cubic symmetry appearing in the four-spin correlation function. Experiments on structural phase transitions are considered briefly.

Many magnetic materials have single-ion terms in the Hamiltonian which reflect the lattice symmetry and so break full rotational invariance.[1] Such terms are also needed to describe structural phase transitions.[2] For a lattice of cubic symmetry, the lowest-order single-ion terms have the form

$$\mathcal{H}_c = v_1 \sum_\alpha \sum_{\vec{R}} (S^\alpha_{\vec{R}})^4, \tag{1}$$

where $S^\alpha_{\vec{R}}$ ($\alpha = 1, 2, \ldots, n$) is the α component of the spin vector $\vec{S}_{\vec{R}}$ at the lattice point $\vec{R}$, while v_1 is a constant. The sign of v_1 determines whether the spins tend to align along the cubic axis ($v_1 < 0$), or in the diagonal (1, 1, 1, ...) directions ($v_1 > 0$). We discuss here mainly the case $v_1 > 0$, since for $v_1 < 0$ a first-order transition is indicated in zero field,[3] and a different approach may be needed.

With the aid of Wilson's renormalization-group approach,[4] and the $\epsilon = 4 - d$ expansion technique,[5] this problem may, for the first time, be attacked seriously. In fact, Wilson and Fisher[5] considered the Hamiltonian (1) for $n = 2$, and concluded that in this case there exists an additional Ising-like fixed point. As we shall emphasize in the present note, the case $n = 2$ is special, and for all $n > 2$ this additional fixed point leads to a new cubic-symmetry-dominated critical behavior. Although the present study, to order ϵ^2, leads to small changes in the critical exponents for $n = 3$ and $\epsilon = 1$ [see Eq. (15) below], it shows that there are appreciable changes in the behavior of the four-spin correlation function, and emphasizes the possible existence of distinct exponents for systems with only cubic symmetry. The accuracy of the ϵ expansion is probably not very great when $\epsilon = 1$, and the actual values of these new exponents should be sought by experiment. In other studies, Cowley and Bruce[6] (for $n = 3$) and Wegner[7] (for general n) have studied the stability of the Heisenberg fixed point (with $v_1 = 0$) with respect to perturbations of the form (1). To order ϵ, they conclude that the fixed point is stable for $n = 3$. As we shall see in the present note, the problem of stability is complicated, and to order ϵ^2 the new cubic fixed point becomes stable and determines the critical behavior. None of the previous studies considered this cubic critical behavior.

Terms of cubic symmetry may also enter the Hamiltonian through exchange interactions. To second order in the momentum $\vec{q}$, the exchange terms have the general form

$$\mathcal{H}_{ex} = -\int_{\vec{q}} \sum_\alpha [J - J_1 q^2 - J_2 (q^\alpha)^2] S^\alpha_{\vec{q}} S^\alpha_{-\vec{q}}. \tag{2}$$

The parameter J_2 evidently measures departures from full rotational invariance. It is related to v_1 via the renormalization-group recursion relations which generate terms like (1) and (2), even if v_1 vanishes initially.[8] Since the J_2 term couples space and spin coordinates, one must take $n = d = 4 - \epsilon$. However J_2 then turns out to be an irrelevant variable for all u_1, $v_1 > 0$ (where u_1 is the coefficient of $\sum_{\vec{R}} S^4_{\vec{R}}$),[8] which decays very slowly (with exponent of order ϵ^2, if u_1, v_1 are of order ϵ). The parameter which leads to instabilities of the fixed point is v_1; accordingly, we restrict the remainder of the discussion to $\mathcal{H}_c$ given by (1) (with general n). However, since J_2 decays so slowly, it may affect many experimental measurements.[9]

The relative magnitude of the anisotropic terms can be measured by

$$v = v_1 kT/J^2, \tag{3}$$

where J is an average exchange coupling [see (2)]. The relative shift of the critical temperature, with respect to its "isotropic" value, is expected to be of order v, and if $v \ll 1$, the usual isotropic behavior should be observed when T is not close to T_c. However, since the Hamiltonian (1) breaks rotational invariance, it is reasonable to expect[10] some new, characteristically cubic-symmetric, behavior to appear for $t = (T - T_c)/T_c \leq t^\times = v^{1/\phi}$, where ϕ is an appropriate crossover exponent.[11]

The main computation uses the exact renormalization-group equations[12] for a reduced Hamiltonian of the form

$$\bar{\mathcal{H}} = -\frac{1}{2}\int_{\vec{q}} (r+q^2)\sum_\alpha S^\alpha_{\vec{q}}\cdot S^\alpha_{-\vec{q}} - \sum_{\alpha\beta}(u+v\delta_{\alpha\beta}) \times \int_{\vec{q}}\int_{\vec{q}'}\int_{\vec{q}''} S^\alpha_{\vec{q}} S^\alpha_{\vec{q}'} S^\beta_{\vec{q}''} S^\beta_{-\vec{q}-\vec{q}'-\vec{q}''}, \quad (4)$$

where $\int_{\vec{q}}$ means $(2\pi)^{-d}\int d^dq$. As usual, r is proportional to $(T-T_0)$, while the coefficient of q^2 is fixed at unity by a spin recaling.

Assuming a small momentum cutoff, b^{-1}, one may ignore all the "mass-renormalization" Feynman graphs and all the irrelevant parameters, and keep only terms of order $\ln b$ in the recursion relations. The recursion relations for u and for v now become

$$u' = b^{\epsilon-2\eta}\{u - 4K_d \ln b(1+\tfrac{1}{2}\epsilon\ln b)[(n+8)u^2+6uv] + 16K_4^2\ln^2 b[(n^2+6n+20)u^3+9(n+4)u^2v+27uv^2] + 32K_4^2\ln b(1+\ln b)[(5n+22)u^3+36u^2v+9uv^2]\}, \quad (5)$$

$$v' = b^{\epsilon-2\eta}\{v - 4K_d\ln b(1+\tfrac{1}{2}\epsilon\ln b)(12uv+9v^2) + 16K_4^2\ln^2 b(36u^2v+54uv^2+27v^3) + 32K_4^2\ln b(1+\ln b)[3(n+14)u^2v+72uv^2+27v^3]\}, \quad (6)$$

where

$$\eta = 8K_4^2[(n+2)u^2+6uv+3v^2]. \quad (7)$$

These recursion relations have four fixed points:

Gaussian:

$$u^G = v^G = 0;$$

Ising:

$$u^I = 0,\ v^I = \frac{\epsilon}{36K_d}(1+\tfrac{17}{27}\epsilon) + O(\epsilon^3);$$

Heisenberg:

$$v^H = 0,\ u^H = \frac{\epsilon}{4K_d(n+8)}\left(1+\frac{3(3n+14)}{(n+8)^2}\epsilon\right) + O(\epsilon^3);$$

Cubic:

$$u^C = \frac{\epsilon}{12K_d n}\left(1+\frac{(n-1)(106-19n)}{27n^2}\epsilon\right) + O(\epsilon^3),$$

$$v^C = \frac{\epsilon}{12K_d n}\left(\frac{n-4}{3}+\frac{(n-1)(17n^2+110n-424)}{8\ln^2}\epsilon\right) + O(\epsilon^3).$$

Note that the Gaussian and Ising fixed points are independent of n.

The (eigenvalue) exponents λ_u and λ_v [Wegner's[7] $(d-x_{2s})$ and $(d-x_{0g})$] for the first three fixed points are[13]

Gaussian:

$$\lambda_u^G = \lambda_v^G = \epsilon;$$

Ising:

$$\lambda_u^I = \tfrac{1}{3}\epsilon - \tfrac{19}{81}\epsilon^2 + O(\epsilon^3),\quad \lambda_v^I = -\epsilon + \tfrac{17}{27}\epsilon^2 + O(\epsilon^3);$$

Heisenberg:

$$\lambda_u^H = -\epsilon + \frac{9n+42}{(n+8)^2}\epsilon^2 + O(\epsilon^3),$$

$$\lambda_v^H = \frac{n-4}{n+8}\epsilon + \frac{5n^2+14n+152}{(n+8)^3}\epsilon^2 + O(\epsilon^3).$$

Note that for $n=1$, we have $v^I = u^H$ and $\lambda_v^I = \lambda_u^H$, as expected. The exponent λ_u^H is related to the leading correction to scaling, discussed by Wegner[14] to order ϵ. We now consider the values of these exponents at $\epsilon=1$ ($d=3$). Although ϵ expansions usually give reasonable results at $\epsilon=1$ on truncation at order ϵ^2, this approach is not always clearly justified; we shall return to this question later. For $\epsilon=1$, the Gaussian and the Ising fixed points are clearly unstable ($\lambda>0$). The stability of the Heisenberg fixed point depends on n: For large values of n it is clear that $\lambda_v^H>0$, and the Heisenberg fixed point is unstable with respect to the cubic perturbation. Thus, the spherical-model limit ($n\to\infty$) of the usual isotropic fixed point is also unstable, and it would be interesting to study a new type of a "cubic spherical model." The borderline of stability of the Heisenberg fixed point depends on the order of the truncated series used for λ_v^H. Using the order-ϵ result, the Heisenberg fixed point is stable for $n<4$. This explains Cowley and Bruce's[6] result for $n=3$. Using the order-ϵ^2 expression, given above, one finds that $\lambda_v^H>0$ for $n>2$, and $\lambda_v^H=0$ at $n=2$. Recently, Ketley and Wallace[15] calculated the order-ϵ^3 term in λ_v^H, using a Feynman-graph expansion near the Heisenberg fixed point. To that order, they find the borderline goes up and lies close to $n=4$. Ketley and Wallace conclude that for $n=3$ the radius of convergence of the series for λ_v^H is smaller than 1, and that no conclusions may be drawn. We conclude tentatively that λ_v^H is either positive or very small in magnitude, so that it is important to study other possible fixed points and other types of critical behavior.[16]

We thus discuss the stability of the cubic fixed point. We must linearize Eqs. (5) and (6) around the fixed-point values, and diagonalize the 2×2 matrix of the coefficients. The results are

$$\lambda_1^C = -\epsilon + \frac{(n-1)(17n^2-4n+212)}{27n^2(n+2)}\epsilon^2 + O(\epsilon^3) \quad (8)$$

and

$$\lambda_2^C = \frac{4-n}{3n}\,\epsilon + \frac{(n-1)(19n^3 - 72n^2 - 660n + 848)}{81n^3\,(n+2)}\,\epsilon^2 + O(\epsilon^3). \tag{9}$$

Note that for $n = 1$ the cubic fixed point is degenerate with the Gaussian fixed point, with $\lambda_2 = \lambda^G = \epsilon$. For $n = 2$ it is degenerate with the Ising fixed point $\lambda_1^C = \lambda_v^I$, $\lambda_2^C = \lambda_u^I$), as predicted by Wilson and Fisher.[3] For $n = 3$ we find

$$\lambda_1^C = -\epsilon + 0.581\epsilon^2 + O(\epsilon^3), \qquad \lambda_2^C = \tfrac{1}{9}\,\epsilon - 0.232\epsilon^2 + O(\epsilon^3). \tag{10}$$

Thus, to order ϵ^2, the cubic fixed point is stable for $n = 3$ at $\epsilon = 1$. It is clearly also stable for all $n > 3$.

Near the Heisenberg fixed point, the correlation length $\xi(t, v)$ scales with v/t^ϕ, with the crossover exponent

$$\phi = \nu^H \lambda_v^H. \tag{11}$$

For $n = 3$, $\epsilon = 1$, $1/\phi \simeq 18$, and hence one should observe cubic symmetric behavior only for rather small values of t, unless $v \gtrsim 1$. Even when $\lambda_v^H < 0$ and $|\lambda_v^H| \ll 1$, one will approach the real Heisenberg critical region only for very small values of t, and feel the cubic effects for all other values.

To find the critical exponent ν^C we turn to the recursion formula for the temperature parameter r. With the same assumptions as before Eq. (5), this recursion formula is

$$r' = b^{2-\eta}\{r + 4K_d[(n+2)u + 3v]A(r) - 32K_4^2[(n+2)u^2 + 6uv + 3v^2]B(r) + \cdots\}, \tag{12}$$

where $A(r)$ and $B(r)$ are the usual integrals over the propagator. Substituting these integrals, and linearizing about a fixed point, yield the exponent ν,

$$\frac{1}{\nu} = \lambda = \frac{\ln\Lambda}{\ln b} = 2 - \eta - 4K_d[(n+2)u^* + 3v^*] + 48K_4^2[(n+2)u^{*2} + 6u^*v^* + 3v^{*2}]. \tag{13}$$

For the cubic fixed point we now find, from (7) and (13),

$$\eta^C = \frac{(n+2)(n-1)}{54n^2}\,\epsilon^2 + O(\epsilon^3), \tag{14}$$

$$2\nu^C = 1 + \frac{n-1}{3n}\,\epsilon + \frac{n-1}{324n^3}\,(17n^2 + 290n - 424)\epsilon^2 + O(\epsilon^3). \tag{15}$$

These may be compared with the Heisenberg-like exponents given in Refs. 5 and 12.

Unfortunately, for $n = 3$ and $\epsilon = 1$ one finds $\nu^C \simeq 0.680$ and $\nu^H \simeq 0.678$, so that to order ϵ^2 it is very difficult to distinguish between these two exponents. The most important conclusion, however, is that a crossover and new values of the exponents are to be expected. In addition, the critical correlation functions should display some features of cubic symmetry arising in part from terms like J_2 in (2)[9] (which may have a nonzero fixed-point value, of order ϵ^3). The fact that v has a nonzero fixed-point value is directly detectable in the four-spin correlation function, which, to lowest order, now has the form

$$\langle S_0^\alpha S_0^\alpha S_0^\beta S_0^\beta \rangle_C \propto (u^C + v^C \delta_{\alpha\beta})\, t^{\epsilon/[\text{illegible}]} \,. \tag{16}$$

These new exponents, and the cubic features of the correlations, should be looked for experimentally. Experiments on the structural phase transition in $SrTiO_3$ give $\nu = 0.63 \pm 0.07$,[9] but the errors are too large for a meaningful comparison. Other experiments give $\beta = 0.333 \pm 0.10$,[18] which might be significantly different from the Heisenberg value $\beta = 0.37 \pm 0.01$.[19] Note that the experiments give $\beta^C < \beta^H$, while we predict $\beta^C > \beta^H$. This may be due to the truncation of our results at ϵ^2.

Another cause for a possible disagreement of the theory with the results on $SrTiO_3$ lies in the experimentally large value of J_2: J_2/J_1 is of the order unity.[9] For small values of J_2/J_1, it has been demonstrated[13] that J_2 is irrelevant and that its exponent is of order ϵ^2. For large values of J_2/J_1, Cowley and Bruce also indicate that J_2 is irrelevant.[6] Thus, one has to be very close to T_c for J_2 to decay to zero.

In any event, we believe the present theory should be more appropriate for the problem of structural phase transitions than the $n = 2$ Heisenberg model suggested by Stanley,[20] since it directly uses the lattice symmetry of the Hamiltonian.

The author is indebted to Professor Michael E. Fisher and to Professor Kenneth G. Wilson for advice and discussions. The support of the National Science Foundation, partly through the Materials Science Center at Cornell University, and a scholarship received from the Fulbright-Hays Committee, are gratefully acknowledged. Comments from Dr. Morgan Grover improved the final form of the manuscript.

[1]For a review of magnetic Hamiltonians, see F. Keffer, in *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, 1966), Vol. XVIII, Pt. 2, p. 1.

[2]K. A. Müller, in *Structural Phase Transitions and Soft Modes*, edited by E. J. Samuelsen, E. Andersen, and J. Feder (Universitetsforlaget, Oslo, 1971), pp. 61 and 73.

[3]W. Corchran, in Ref. 2, p. 1; D. J. Wallace, J. Phys. C **6**, 1390 (1973); K. G. Wilson and M. E. Fisher, Phys. Rev. Lett. **28**, 240 (1972), and private communication.

[4]K. G. Wilson, Phys. Rev. B **4**, 3174 (1971); Phys. Rev. B **4**, 3184 (1971).

[5]K. G. Wilson and M. E. Fisher, Phys. Rev. Lett. **28**, 240

(1972); K. G. Wilson, Phys. Rev. Lett. **28**, 548 (1972).

[6]R. A. Cowley and A. D. Bruce, J. Phys. C 6, L191 (1973).

[7]F. J. Wegner, Phys. Rev. B **6**, 1891 (1972).

[8]M. E. Fisher and A. Aharony, Phys. Rev. Lett. 30, 559 (1973); A. Aharony and M. E. Fisher, Phys. Rev. B 8, 3323 (1973); A. Aharony, Phys. Rev. B 8, 3349 (1973).

[9]Th. von Waldkirch, K. A. Müller, W. Berlinger, and H. Thomas, Phys. Rev. Lett. **28**, 503 (1972); Th. von Waldkirch, K. A. Müller, and W. Berlinger, Phys. Rev. B **7**, 1052 (1973).

[10]M. E. Fisher, Rep. Prog. Phys. **30**, 615 (1967).

[11]E. K. Riedel and F. Wegner, Z. Phys. **225**, 195 (1969); D. Jasnow and M. E. Fisher, *Theory of Critical Correlations* (Academic, New York, to be published).

[12]K. G. Wilson and J. Kogut, Phys. Rept. (to be published).

[13]A. Aharony, Phys. Rev. B 8, 3349 (1973). Note that the dependence of η on u and on v, Eq. (7), has to be taken into account in linearizing (5) and (6). I thank Professor David Wallace for this comment.

[14]F. J. Wegner, Phys. Rev. B **5**, 4529 (1972). See also A. Aharony, Phys. Rev. B 8, 3349 (1973). The eigenvalue λ_v^H has also been calculated to order ϵ^3 using the Callan-Symanzik approach, and the results to order ϵ^2 agree with ours [E. Brézin, J. C. Le Guillou, and J. Zinn-Justin, Phys. Rev. B (to be published)].

[15]I. J. Ketley and D. J. Wallace (report of work prior to publication).

[16]It may be mentioned that a numerical study (Ref. 17) at $n = 3$, $d = 3$ of the approximate recursion relations gives $\lambda_v^H = -0.053$, which is smaller in magnitude than the order ϵ result, but is still negative. The range of validity of the approximate recursion relations is not clear, and therfore this result only strengthens our feeling that the other possiblilties have to be investigated.

[17]M. K. Grover, L. P. Kadanoff, and F. J. Wegner, Phys. Rev. B **6**, 311 (1972).

[18]K. A. Müller and W. Berlinger, Phys. Rev. Lett. **26**, 13 (1971).

[19]M. J. Cooper, M. Vincentini-Missoni, and R. I. Joseph, Phys. Rev. Lett. **23**, 70 (1969).

[20]H. E. Stanley, in Ref. 2, p. 271.