PHYSICAL REVIEW LETTERS

VOLUME 37 — 6 SEPTEMBER 1976 — NUMBER 10

Magnetization of Cubic Ferromagnets and the Three-Component Potts Model

David Mukamel, Michael E. Fisher, and Eytan Domany
Baker Laboratory and Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853
(Received 19 April 1976)

The (H_x, H_y, H_z) phase diagram of a cubic ferromagnet with three easy axes, in a field $\vec{H}=(H_x, H_y, H_z)$, is studied by mean-field, scaling, and renormalization-group theories. For $T < T_c(H=0)$ and $\vec{H} \parallel [111]$ there is a phase transition at fields $\pm H_0(T)$, described by the three-component Potts model. By varying $\vec{H}$ the full phase diagram of the three-dimensional Potts model is experimentally accessible and competing predictions of the multicritical behavior can be tested.

The magnetization of a ferromagnetic crystal with cubic anisotropy is an old topic which has been studied[1-4] since 1926. But, as we will show, a variety of phase transitions and multicritical points should occur in low magnetic fields, $\vec{H}$ (of order $H_{\rm Aniso}$), which seem to have been overlooked in previous theoretical work and, so far, unseen experimentally. Furthermore, it transpires that in a "diagonal" field, $\vec{H} \parallel [111]$, cubic ferromangets with three easy axes, [100], [010], and [001], such as Fe, $PrAl_2$, $NdAl_2$, etc.,[3,4] provide experimentally accessible realizations of a three-dimensional, $(q=3)$-component Potts model,[5] which is currently a system of appreciable theoretical interest.[6-11]

High-temperature series extrapolation studies[6] and exact analytic calculations of the latent heat[7] have shown that the $(d=2)$-dimensional Potts model exhibits a *continuous* phase transition (in zero symmetry-breaking field) when $q \leq 4$. On the other hand,[6] when studied phenomenologically the free energy of the $q=3$ Potts model contains a term of third degree in the order parameter and hence, in accord with Landau theory, the transition is predicted to be of *first* order! Approximate renormalization-group calculations for $d=3$, and exact work for small $\epsilon = 4-d$, likewise indicate a first-order transition.[9] (These renormalization-group studies utilize a continuous spin version of the Potts model but, on the usual grounds of universality, the critical and multicritical behavior is expected to be the same as for the original discrete-state model.)

The three-dimensional $q=3$ Potts model has been studied by series expansions,[11] but conflicting conclusions have been reached. To decide if the transition in three dimensions is continuous (as for $d=2$) or is first order (as, presumably, for $d \geq 4$) it is of interest to find real systems which may be described by the Potts Hamiltonian. In fact, it is not hard to see that a cubic ferromagnet with three easy axes provides a rather accurate realization of a $q=3$ Potts model. In the remainder of this note we substantiate this picture in more detail and discuss various explicit predictions for the phase diagram on the basis of mean-field theory, scaling concepts, and renormalization-group analysis.

Certain basic features of the phase diagram follow quite generally from the cubic symmetry and the existence of six equivalent easy directions of magnetization in zero field. A small magnetic field ($|\vec{H}| \ll H_A$) will merely stabilize that easy direction of magnetization which lies closest to the direction of $\vec{H}$. As $\vec{H}$ passes through the planes (110), (101), etc., the appropriate easy direction

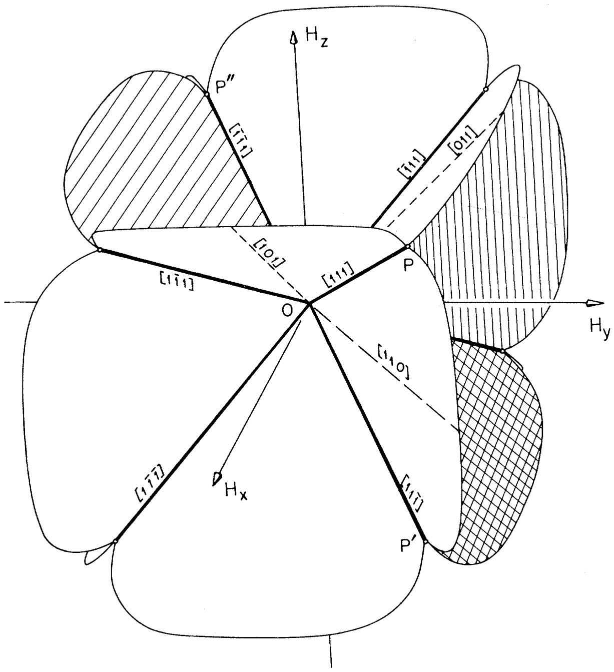

FIG. 1. View in (H_x, H_y, H_z) space of the schematic phase diagram of a cubic ferromagnet with three easy axes at fixed T below T_c, drawn in accord with results for the two-dimensional $q=3$ Potts model. Bold lines denote lines of magnetic triple points; thin curves represent critical lines of Ising character; the open circles labeled P, P', etc., mark the "anomalous tricritical" or Potts points.

switches and the system hence undergoes a first-order transition. Thus, as illustrated in Fig. 1, the space (H_x, H_y, H_z) is divided, for small H, into six regions by twelve first-order planes. These planes meet on the principal diagonals, [111], etc. (shown bold in Fig. 1), where the three distinct magnetic phases, related to one another by a threefold rotation, are in equilibrium. These three phases correspond to the ordered states of the $q=3$ Potts model.

The first-order surfaces must, in larger fields $(|\vec{H}| \simeq H_A)$, terminate in critical edges, i.e., lines of critical points (which should be Ising like in character). Indeed, for large $\vec{H} \parallel [111]$ the magnetization $\vec{M}$ will be parallel to $\vec{H}$; the two components of $\vec{H}$ orthogonal to [111] correspond to the two ordering fields, h_1 and h_2, for the Potts model.[6] Since the relevant fields may be small ($H_A \simeq 400$ Oe for Fe) the whole phase diagram of a $q=3$ Potts model can be explored experimentally in a real cubic ferromagnet.[12]

The simplest topology for the critical edges is illustrated in Fig. 1. Three critical lines meet on each diagonal at an *anomalous* tricritical point,[6] or Potts point, labeled P, P', etc. In the vicinity of a Potts point, the $\vec{H}$ phase diagram has the same form as that of the *two*-dimensional, $q=3$ Potts model in (T, h_1, h_2) space.[6] However, mean-field and Landau theories do *not* yield Potts points.

To show the equivalence of the ferromagnet to a $q=3$ Potts model more formally, we may consider the Landau-Ginzburg-Wilson Hamiltonian for a continuous $(n=3)$-component spin field $\vec{s}(\vec{R})$ in a reduced magnetic field $\vec{h} = m\vec{H}/k_B T$. For a cubic ferromagnet the local terms are

$$U(\vec{s}) = -\vec{h}\cdot\vec{s} + \tfrac{1}{2} r|\vec{s}|^2 + u|\vec{s}|^4 + v(s_x^4 + s_y^4 + s_z^4). \qquad (1)$$

Stability requires $u+v>0$ and, for the anisotropy, we take $v<0$ which yields the desired three easy axes.[13] An orthogonal transformation $\vec{s} \to \vec{\sigma} = (\sigma_0, \sigma_1, \sigma_2)$, with $\sigma_0 \propto s_x + s_y + s_z$ and $\sigma_1 \propto s_x - s_y$, takes U into the same form except that the last term becomes

$$\tfrac{1}{3}v[6\sigma_0^2(\sigma_1^2 + \sigma_2^2) - 2\sqrt{2}\sigma_0(\sigma_2^3 - 3\sigma_1^2\sigma_2) + \tfrac{3}{2}(\sigma_1^2 + \sigma_2^2)^2 + \sigma_0^4]. \qquad (2)$$

Now fix $T < T_c(0)$ so that $r<0$, and vary the diagonal field $\vec{h} = (h_0, h_1 = 0, h_2 = 0)$. For large $\vec{h}$ the spin component σ_0 is noncritical and may hence be replaced by its mean value $\bar{\sigma}_0(h_0)$, while, by symmetry $\langle\sigma_1\rangle = \langle\sigma_2\rangle = 0$. However, as h_0 is reduced, the components σ_1 and σ_2 become critical when $\tilde{r}(\bar{\sigma}_0) = r + 4(u+v)\bar{\sigma}_0^2 \approx a h_0 - b|v|$ vanishes. The system may then be described in terms of the reduced, *two*-component order parameter, $\vec{\Psi} = (\sigma_1, \sigma_2)$, with a reduced Hamiltonian of the same form as (1) but with last term given by $\tilde{v}(\bar{\sigma}_0)(\Psi_2^3 - 3\Psi_1^2\Psi_2)$; but such a coupling merely describes the continuous spin version of the $q=3$ Potts model.[9]

On applying[14] mean-field theory to (1) we find[13] that the phase diagram below T_c for $|v|/(u+v) < 2$ (i.e., small anisotropy) has the form shown schematically in Fig. 2 [see also Fig. 3(a)]. As found by Straley and Fisher,[6] the Potts point P of Fig. 1 is replaced by a quadruple point, Q, lying on the [111] diagonal (and likewise in other octants). At Q *four* distinct phases are in equilibrium. Varying $\vec{H} \parallel [111]$ through Q yields a *first-order* phase transition with a jump in $|\vec{M}|$ [see Fig. 3(b)].

The critical edges of the original first-order planes now terminate (see Fig. 4) in three sym-

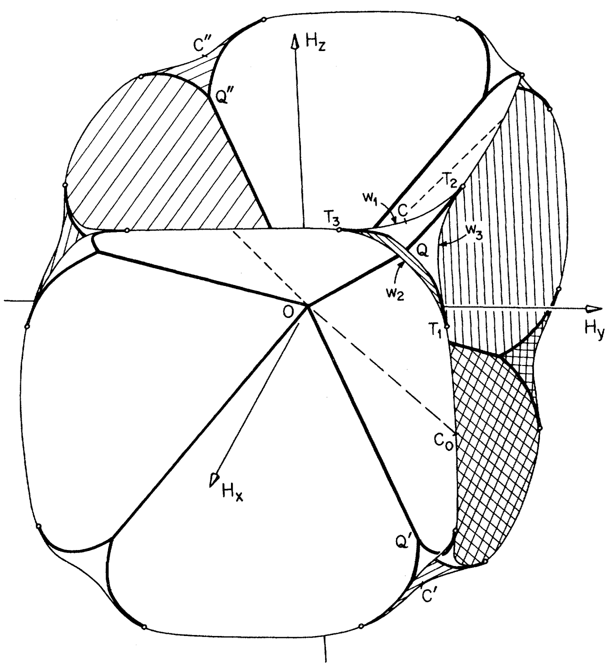

FIG. 2. Schematic phase diagram drawn in accord with mean-field and Landau theories. All critical lines (thin) including the "wings," w_1, w_2, and w_3, should be of Ising character; C and C_0 are particular critical points; T_1, T_2, and T_3 denote a trio of *tri*critical points (open circles). Four lines of triple points (bold) meet at each of the quadruple points Q, Q', etc.

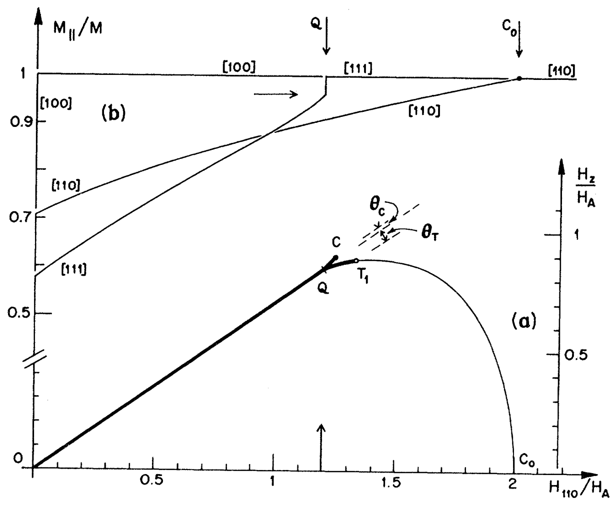

FIG. 3. (a) Section of Fig. 2 in the (H_{110}, H_z) plane (right scale) showing critical points C and C_0, a tricritical point T_1, first-order phase boundaries (bold), and critical lines (thin); (b) corresponding magnetization curves (left scale) according to mean-field theory for $\vec{H}$ parallel to [100], [110], and [111], showing the first-order transition, for [111], at Q and second-order transition (i.e., critical point) at C_0.

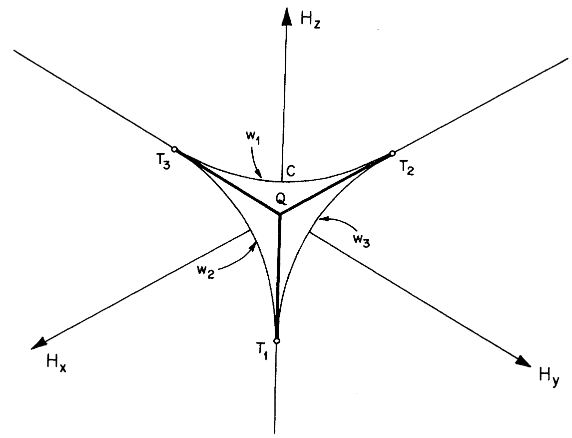

FIG. 4. Partial view down the [111] axis of Fig. 2 showing the tricritical points T_1, T_2, and T_3, the tricritical wings w_1, w_2, and w_3, a critical point, C, in the plane of the H_z axis, and the quadruple point Q.

metrically arranged *tri*critical points, T_1, T_2, and T_3, which are connected by three critical "wings," w_1, w_2, and w_3, bounding new coexistence surfaces which converge on the quadrupole point. The presence of these wing surfaces ensures a first-order transition as a function of field at fixed orientation even if $\vec{H}$ is somewhat misaligned from the three-fold axis (see below).

Important features of the mean-field phase diagram can be determined quantitatively when $v/u \to 0$, simply by minimizing the molecular field energy,

$$E = -\vec{H}\cdot\vec{M} - \tfrac{1}{2}K_1(M_x^{\,4} + M_y^{\,4} + M_z^{\,4})/M_0^{\,4}, \qquad (3)$$

for a ferromagnet with fixed $|\vec{M}| \equiv M_0$ and positive fourth-order anisotropy parameter, $K_1 \propto v$. In the (H_{110}, H_z) or $(1\bar{1}0)$ plane [see Fig. 3(a)], we calculate the following coordinates in units of $H_A = K_1/M_0$: C_0, $(2,0)$; Q, $(1.197, 0.846)$; C, $(1.246, 0.893)$; and T_1, $(1.330, 0.883)$. Hence, we find the opening angles $\theta_C = \angle COQ \simeq 0.36°$ and $\theta_T = \angle T_1OQ \simeq 1.68°$. Of course these mean-field results can be no more than a guide to an experimental study but they suggest that misalignments of up to $\frac{1}{4}°$ may be acceptable. Some corresponding magnetization curves are shown in Fig. 3(b). The first-order transition occurs at $|\vec{H}| = 1.4657H_A$ and the jump in magnetization is 3.666% of M_0. Existing experimental data[1-4] confirm the general shape of these plots but are too sparse to detect the transition.

The standard prediction of general scaling theory[15] for the magnetization of a cubic ferromagnet as $t=(T-T_c)/T_c \to 0$ may be rewritten as

$$\vec{M}(\vec{H}, T) \approx |t|^{\beta} Y(\vec{h}/|t|^{\Delta^*}|v|^{\zeta}, v|t|^{-\varphi_v}), \qquad (4)$$

where $\Delta^* = 2-\alpha-\beta-\zeta\varphi_v$, in which $\alpha \simeq -0.14$ and $\beta \simeq 0.36$ are standard Heisenberg-like ($n=3$) exponents while $\varphi_v \simeq -0.03 < 0$ is the crossover exponent for cubic anisotropy[16]; finally ζ is an *arbitrary* exponent. Above T_c one may, as usual, choose $\zeta=0$ and v is then a standard irrelevant variable[16] which can be neglected as $t\to 0$. Below T_c, however, v is a "dangerous irrelevant variable,"[16,17] which cannot safely be set equal to zero. Nevertheless, in mean-field theory (where $\varphi_v \equiv 0$) the unique choice $\zeta=1$ allows one to set v equal to 0 in the *second* argument of $Y(x,y)$, so that $\vec{M}/|t|^{\beta}$ becomes a function only of $\vec{h}/|v|^{\zeta}|t|^{\Delta^*}$. We expect this result to hold more generally for appropriate $\zeta(d)$. An explicit ϵ-expansion calculation of the critical surfaces[13] yields $\vec{h}_c(T) \sim v|t|^{\psi}$ with $\psi = 2-\alpha-\beta-\varphi_v$; via extended scaling[15] this implies $\zeta(d)\equiv 1$. Consequently we predict that the whole $\vec{H}$ phase diagram scales as $v|t|^{\Delta^*}$ with $\Delta^* \simeq 1.8$.

We thank Dr. P. Bak for helpful discussions and are grateful for the support of the National Science Foundation, in part through the Materials Science Center at Cornell University.

[1] K. Honda and S. Kaya, Sci. Rep. Tohoku Imp. Univ. 15, 721 (1926); H. J. Williams, Phys. Rev. 52, 747 (1937).

[2] See, for example, R.M. Bozorth, *Ferromagnetism* (Van Nostrand, Princeton, N. J., 1951); K. H. Stewart, *Ferromagnetic Domains* (Cambridge Univ. Press, Cambridge, England, 1954); and M. I. Darby and E. D. Isaac, IEEE Trans. Magn. 10, 259 (1974).

[3] W. J. Carr, Jr., in *Encyclopedia of Physics*, edited by H. P. J. Wijn (Springer, Berlin, 1966), Vol. XVIII/2, p. 284.

[4] H. G. Purwins, E. Walker, B. Barbara, M. F. Rossignol, and P. Bak, J. Phys. C 7, 3573 (1974); these authors report some indications of a transition in the region of the expected quadruple or Potts point but we feel that the data presented are not convincing; P. Bak, J. Phys. C 7, 4097 (1974); J. Sznajd, Acta Phys. Pol. A 47, 61 (1975).

[5] R. B. Potts, Proc. Cambridge Philos. Soc. 48, 106 (1952).

[6] J. P. Straley and M. E. Fisher, J. Phys. A 6, 1310 (1973).

[7] R. J. Baxter, J. Phys. C 6, L445 (1973).

[8] S. Alexander and G. Yuval, J. Phys. C 7, 1609 (1974); D. Mukamel and M. Blume, Phys. Rev. A 10, 610 (1974).

[9] G. Golner, Phys. Rev. B 8, 3419 (1973); D. J. Amit, and A. Shcherbakov, J. Phys. C 7, L96 (1974); J. Rudnick, J. Phys. A 8, 1125 (1975).

[10] D. Kim *et al.*, Phys. Rev. B 12, 989 (1975), and 13, 2054 (1976).

[11] R. V. Ditzian and J. Oitmaa, J. Phys. A 7, L61 (1974); J. P. Straley, J. Phys. A 7, 2173 (1974).

[12] It has been suggested that the lattice-gas transition of He adsorbed on Grafoil is described by the zero-field Potts model in $d=2$ dimensions [S. Alexander, Phys. Lett. 54A, 353 (1975)], and that the structural transition in the A-15 compounds provides a realization of the zero-field Potts model in $d=3$ dimensions [M. Weger and I. B. Goldberg, Solid State Phys. 28, 1 (1973)].

[13] D. Mukamel, E. Domany, and M. E. Fisher, to be published, also discuss the cases $v>0$ and $-v/(u+v) > 2$. Previous work (e.g., Refs. 2 and 4) has been restricted to the symmetry axes.

[14] See, for example, S. Krinsky and D. Mukamel, Phys. Rev. B 11, 399 (1975), and 12, 211 (1975).

[15] See M. E. Fisher, in *Proceedings of the Twenty-Fourth Nobel Symposium on Collective Properties of Physical Systems, Aspenaasgarden, Sweden, 1973*, edited by B. Lundqvist and S. Lundqvist (Nobel Foundation, Stockholm, 1973), p. 16; P. Pfeuty, D. Jasnow, and M. E. Fisher, Phys. Rev. B 10, 2088 (1974).

[16] M. E. Fisher, Rev. Mod. Phys. 46, 597 (1974); M. E. Fisher and D. R. Nelson, Phys. Rev. Lett. 32, 1350 (1974); A. D. Bruce and A. Aharony, Phys. Rev. B 11, 428 (1975).

[17] See M. E. Fisher, in *Renormalization Group in Critical Phenomena and Quantum Fields: Proceedings of a Conference*, edited by J. D. Gunton and M. S. Green (Temple Univ. Press, Philadelphia, Pa., 1974); D. R. Nelson, Phys. Rev. B 13, 2222 (1976).