Influence of fluctuations on the magnetisation of cubic ferromagnets

1989 J. Phys.: Condens. Matter 1 8747

(http://iopscience.iop.org/0953-8984/1/44/043)

J. Phys.: Condens. Matter **1** (1989) 8747–8751. Printed in the UK

LETTER TO THE EDITOR

Influence of fluctuations on the magnetisation of cubic ferromagnets

Marcia C Barbosa† and W K Theumann‡

† Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742, USA

‡ Instituto de Física, Universidade Federal do Rio Grande do Sul, Caixa Postal 15051, 91500 Porto Alegre, RS, Brazil

Received 7 June 1989

Abstract. Renormalisation-group calculations to first order in ε, in $4-\varepsilon$ dimensions, for the three-state Potts model are used to study the effects of fluctuations on the phase transition of cubic ferromagnets either in a diagonal or a slightly off-diagonal magnetic field. It is found that these compete with the effects of sixth-order anisotropy leaving a discontinuity for the magnetisation of about the same magnitude as that found in 1976 by Mukamel, Fisher and Domany. Our results may be relevant to the phase transition in $PrAl_2$ and $DyAl_2$ when the temperature is not too low.

The phase transition in cubic ferromagnets with three easy axes, [100], [010] and [001], such as Fe, $NdAl_2$ and $DyAl_2$ (Carr 1966, Purwins *et al* 1974, Bak 1974) in a diagonal magnetic field $\boldsymbol{H} \parallel [111]$, became of considerable interest some time ago (Mukamel *et al* 1976, Barbara *et al* 1978) with the proposal of Mukamel *et al* (1976) that these systems are physical realisations of the three-state Potts model (Potts 1952). There has been a prolonged controversy as to whether the model in three dimensions has a first-order or a continuous transition and there is now strong evidence in support of a first-order transition (Wu 1982). Except for Fe (Hathaway and Prinz 1981), the experimental and theoretical results on cubic ferromagnets are not that definite.

Mean-field calculations (Mukamel *et al* 1976), which hold apparently for all temperatures T, yield a discontinuity in the diagonal magnetisation $\Delta M_{\parallel}$ of only 3.666% of the $T = 0$ value of $M_0 = |\boldsymbol{M}|$, the magnitude of the magnetisation. Experiments on $PrAl_2$ (Purwins *et al* 1974) show a discontinuity of about this size, whereas the discontinuity for $NdAl_2$, if any, is expected to be very small (Bak 1974).

Sixth-order anisotropy is important in rare-earth systems, and it has been argued that this accounts for the larger discontinuities in $DyAl_2$ at low T (Barbara *et al* 1978). It has also been suggested by Barbara *et al* (1978) and shown explicitly by Cullen and Callen (1984, 1985) that for cubic ferromagnets with fourth- *and* sixth-order anisotropy the latter *could* increase the off-diagonal angle θ_t where a tricritical point is expected to appear following the increase of the discontinuity in the magnetisation. Although the experiments on $DyAl_2$ at 4.2 K yield a result in the interval $10° < \theta_T < 22.9°$, much larger than the $\theta_T \simeq 1.68°$ of Mukamel *et al* (1976), data indicate that $\theta_T < 10°$ already at 20 K or higher and such small values are probably difficult to detect.

0953-8984/89/448747 + 05 $02.50

Thus, except for $DyAl_2$ at low T (<20 K), the experimental evidence suggests that the phase transition in cubic ferromagnets in a diagonal magnetic field is only weakly first order. Fluctuation corrections near a second-order phase transition (Wilson and Kogut 1974, Fisher 1974) may then be relevant, and in this Letter we show that renormalisation-group (RG) calculations also yield off-diagonal tricritical *and* critical angles that vary in proportion to the discontinuity in the magnetisation in a *non*-trivial way. A classical mean-field calulation that includes sixth-order anisotropy near a second-order phase transition is then shown to yield results that *compete* with the fluctuation corrections.

A cubic ferromagnet in an external magnetic field can be described by the Landau–Ginzburg–Wilson Hamiltonian

$$\mathcal{H} = \int \mathrm{d}^3x \, \{\tfrac{1}{2}[r_0\psi^2 + (\nabla\boldsymbol{\psi})^2] + u_0(\boldsymbol{\psi}^2)^2 + v_0(\psi_x^4 + \psi_y^4 + \psi_z^4) - \boldsymbol{h}\cdot\boldsymbol{\psi}\} \tag{1}$$

for a continuous three-component field $\boldsymbol{\psi}(\boldsymbol{x}) = (\psi_x, \psi_y, \psi_z)$. The reduced magnetic field $\boldsymbol{h} = m\boldsymbol{H}/k_\mathrm{B}T$, m being the magnetic moment and $\boldsymbol{H}$ the applied magnetic field. Stability requires that $u_0 + v_0 > 0$ and, in order to have the three easy axes [100], [010] and [001] we follow Mukamel *et al* (1976) and take $v_0 < 0$. For our purposes we let $\boldsymbol{h} = h_0(1+\delta, 1+\delta, 1-2\delta)/\sqrt{3}$ and assume $\delta \ll 1$.

The orthogonal transformation to the new field $\boldsymbol{\phi}(\boldsymbol{x}) = (\phi_0, \phi_1, \phi_2)$

$$\begin{aligned}
\phi_0 &= (1/\sqrt{3})[(1+\delta)\psi_x + (1+\delta)\psi_y + (1-2\delta)\psi_z] \\
\phi_1 &= (1/\sqrt{6})[(1-2\delta)\psi_x + (1-2\delta)\psi_y - 2(1+\delta)\psi_z] \\
\phi_2 &= 1(/\sqrt{2})(\psi_x - \psi_y)
\end{aligned} \tag{2}$$

and the separation $\phi_0 = \tilde{\phi}_0 + M_0$, where $M_0 = \langle\phi_0\rangle$ is the thermal average of ϕ_0 and $\tilde{\phi}_0$ is its fluctuating part, yields an intermediate Hamiltonian $\mathcal{H}$ with linear terms in $\boldsymbol{\phi}$: $-\tilde{h}_0\phi_0 - h_1\phi_1$, where

$$\tilde{h}_0 = h_0 - r_0M_0 - 4(u_0 + v_0/3)M_0^3 \tag{3a}$$

$$h_1 = (8\sqrt{2}/3)|v_0|M_0^3\delta. \tag{3b}$$

Then $\langle\tilde{\phi}_0\rangle = 0$ yields $M_0 = M_0(h_0)$.

We follow Mukamel *et al* (1976) and fix $T < T_\mathrm{c}(0)$, the critical temperature in zero field h_0, and vary h_0. For large $h_0 \gg h_\mathrm{a}$, the reduced anisotropy field $(8|v_0|M_0^3)$, ϕ_0 is non-critical and may be replaced by M_0 while, by symmetry $\langle\phi_1\rangle = \mathrm{O}(\delta)$ and $\langle\phi_2\rangle = 0$. The part of $\mathcal{H}$ which does not contain $\tilde{\phi}_0$ becomes the effective Hamiltonian

$$\begin{aligned}
\mathcal{H}_{\mathrm{eff}} = \int \mathrm{d}^3x \, \{&\tfrac{1}{2}[r_1\phi_1^2 + r_2\phi_2^2 + (\nabla\boldsymbol{\phi})^2] + w_1\phi_1^3 - 3w_2\phi_1\phi_2^2 + u_1(\phi_1^2 + \phi_2^2)^2 \\
&+ u_2(\phi_1^4 + \phi_1^2\phi_2^2) - h_1\phi_1\}
\end{aligned} \tag{4}$$

for the three-state Potts model with symmetry-breaking terms which has been previously applied to the trigonal–pseudo-tetragonal phase transition in $SrTiO_3$ (Barbosa and Theumann 1988, 1989). The parameters

$$
\begin{aligned}
r_1 &= r + g & r_2 &= r - g \\
w_1 &= w + 3g_w & w_2 &= w - g_w \\
u_1 &= u - (y + \tfrac{1}{3}z) & u_1 + u_2 &= u + y - \tfrac{1}{3}z
\end{aligned}
\tag{5}
$$

are related to those of the cubic system through

$$r = 8(h_0/h_A - \tfrac{1}{3})|v_0|M_0^2 \tag{6a}$$

$$g = -8|v_0|M_0^2\delta \tag{6b}$$

$$w = (2\sqrt{2/3})|v_0|M_0 \tag{6c}$$

$$g_w = -2\sqrt{2}|v_0|M_0\delta \tag{6d}$$

$$u = |v_0|(h_0/h_A + \tfrac{7}{6}) \tag{6e}$$

$$y = -\tfrac{14}{3}|v_0|\delta \tag{6f}$$

$$z = 2|v_0|\delta. \tag{6g}$$

As h_0/h_A is reduced either ϕ_1 or ϕ_2 start to order and the mean-field phase diagram (Blankschtein and Aharony 1980, Fontanari and Theumann 1986) may then be used to locate the critical and tricritical points.

Renormalisation-group equations for the three-state Potts model with symmetry-breaking perturbations in $d = 4 - \varepsilon$ dimensions have been derived and applied in a different context (Barbosa and Theumann 1988, 1989). They will now be used to obtain the fluctuation corrections to the discontinuity in the magnetisation. In conformity with Mukamel *et al* (1976), we take v_0/u_0 small so that $0 < w^2/u \ll 1$ in the RG equations (Blankschtein and Aharony 1980).

Since by (3*b*) we have $h_1 = O(\delta)$, we consider the ordering of the component ϕ_1 when $\delta \to O^-$ so that $r_1 < r^2$ in (5). Writing $\phi_1 = \tilde{\phi}_1 + M_1$ and $\phi_2 = \tilde{\phi}_2$, where $\tilde{\phi}_1$ and $\tilde{\phi}_2$ are the fluctuating parts in which $M_1 = \langle\phi_1\rangle$, we calculate the latter from the singular part of the free-energy density (Barbosa and Theumann 1989). However, in contrast to that work, which is restricted to the critical point in a *finite* field h_1, we now need M_1 on the phase boundary where ϕ_1 orders *at* $h_1 = 0$ (Mukamel *et al* 1976, Blankschtein and Aharony 1980). A standard calculation yields

$$\Delta M_1 = M_1 = -(w/2u)(qw^2/2u)^{-\varepsilon/5}. \tag{7}$$

When combined with (6) we get an explicit dependence on the parameters for the cubic systems in terms of M_0 and h_0/h_A, in which the latter is determined by the location of the first-order transition as

$$h_0/h_A \simeq 1.54(2.59|v_0|M_0^2)^{-0.023\varepsilon} - \tfrac{7}{6}. \tag{8}$$

Now, as is usual in cubic systems, the ordering of ϕ_1 will cause a (small) secondary change in $\tilde{\phi}_0$, through the linear terms in $\tilde{\phi}_0$ that are in the intermediate Hamiltonian $\mathcal{H}$ referred to above (Blankschtein and Aharony 1981). Since M_1 appears discontinuously

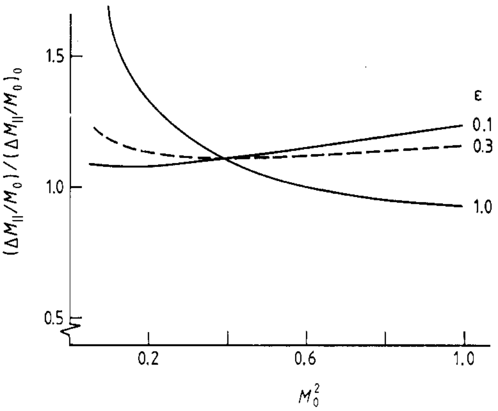

Figure 1. Relative discontinuity of the diagonal magnetisation with respect to its mean-field value as a function of $M_0 = |\boldsymbol{M}|$ for $\varepsilon = 0.1, 0.3$ and 1.0, according to equation (11).

in the Potts model, for the discontinuity in the magnetisation of the cubic system in a *diagonal* field this now yields the result

$$\Delta M_\parallel = \tilde{\phi}_0 \simeq -4(u_0 - |v_0|)M_0 M_1^2/\tilde{r}_0 \tag{9}$$

in which $\tilde{r}_0 = r_0 + 12(u_0 + v_0/3)M_0^3$. A direct calculation using the XY-model fixed-point value for u_0 then yields the estimate for the ratio

$$(\Delta M_\parallel/M_0)/(\Delta M_\parallel/M_0)_0 \simeq (2.59|v_0|M_0^2)^{-0.35\varepsilon} \tag{10}$$

with respect to the mean-field value (the limit $\varepsilon = 0$) found by Mukamel *et al* (1976). Since we are dealing with a first-order transition, it is presumably unjustified to assume (10) to apply when ε is extrapolated far from zero. Noting that $|v_0|M_0^2$ is $O(w^2/u)$, and since $0 < w^2/u \ll 1$, the fluctuation corrections are expected to remain finite. Also, because $\delta = 0$ for a diagonal field, except for the initial cubic anisotropy, symmetry-breaking perturbations play no role in (10). Note that for any reasonable temperature dependence of M_0, fluctuations thus tend to *decrease* the discontinuity as T is lowered.

To estimate the effect of sixth-order anisotropy consider, for simplicity, a single term $s_0(\psi_x^6 + \psi_y^6 + \psi_z^6)$ added to (1) in mean-field theory. Then (10) is modified to

$$(\Delta M_\parallel/M_0)/(\Delta M_\parallel/M_0)_0 \simeq [1 + 0.57(s_0/|v_0|)M_0^2](2.59|v_0|M^2)^{-0.35\varepsilon} \tag{11}$$

and sixth-order anisotropy (with $s_0 > 0$) should thus *increase* the discontinuity as T is reduced, in qualitative agreement with earlier quantum-mechanical, mean-field calculations for $DyAl_2$ (Barbara *et al* 1978). Thus, RG fluctuation corrections that compete with the effect of sixth-order anisotropy could lead to a discontinuity of the same order as that of Mukamel *et al* (1976). This could be the case for $PrAl_2$ as illustrated in figure 1, which represents a numerical estimate of (11) with the choice $|v_0| = 1$ and $s_0 = 0.5$ in accordance with Barbara *et al* (1978). Note that over most of the range of non-zero M_0, to which our calculations are restricted, there is only a change of about 10% to 20% over the already *small* $(\Delta M_\parallel/M_0)_0$. Thus, in cubic ferromagnets when the transition is only weakly first order, sixth-order anisotropy and fluctuation corrections should compete without changing the nature of the transition. In contrast, the low-T experimental results on $DyAl_2$ may be an indication that quantum-mechanical effects force the transition to be entirely first order, with negligible fluctuation corrections.

Before our final comment about the nature of the phase transition in the three-state Potts model, consider the effect of RG fluctuation corrections on the critical and tricritical points in non-zero field h_1, i.e., for $\delta \neq 0$ corresponding to a non-diagonal magnetic field. Using the results of our previous work (Barbosa and Theumann 1988) we find, for the critical and tricritical angles

$$\theta_c/\theta_c^{(0)} \simeq (1.434\,|v_0|M_0^2)^{-0.13\varepsilon} \tag{12}$$

$$\theta_t/\theta_t^{(0)} \simeq (1.437\,|v_0|M_0^2)^{-0.14\varepsilon} \tag{13}$$

respectively. Here quadratic *and* quartic symmetry-breaking terms were included in the calculation of the exponents to ensure that no cancellation takes place. Thus, fluctuation corrections impose the same tendency on the angles as on the discontinuity in the magnetisation. With sixth-order anisotropy taken into account, equations (12) and (13) become modified in a way similar to (11), in agreement with Cullen and Callen (1984, 1985).

Returning to the nature of the phase transition for the three-state Potts model in three dimensions, the consistency of our results with the experiments on $PrAl_2$ and $DyAl_2$ (at not-too-low T) suggests that the transition in the *classical* model is weakly first order. Further experiments and quantum-mechanical calculations are necessary for $DyAl_2$ at rather low T to confirm and explain the apparently large first-order transition.

We thank Professor Michael E Fisher for a critical reading of the manuscript and for suggesting improvements. One of us (MCB) also thanks Professor Fisher for his kind hospitality at the Institute for Physical Science and Technology, University of Maryland, where the work was completed with support through a post-doctoral fellowship from Conselho Nacional de Desenvolvimento Cientifico e Tecnologico (CNPq), Brazil, and an ancillary support through the US National Science Foundation (under Grant No DMR 87-96299). Most of the work was done at Instituto de Física, Universidade Federal do Rio Grande do Sul, Brazil, with partial support from CNPq and from Financiadora de Estudos e Projetos (FINEP). We thank Ronaldo Erichsen for aid in a calculation.

References

Bak P 1974 *J. Phys. C: Solid State Phys.* **7** 4097
Barbara B, Rossignol MF and Bak P 1978 *J. Phys. C: Solid State Phys.* **11** L183
Barbosa M C and Theumann W K 1988 *Phys. Rev.* B **38** 9160
—— 1989 *J. Phys.: Condens. Matter* **1** 6059–70
Blankschtein D and Aharony A 1980 *J. Phys. C: Solid State Phys.* **13** 4635
—— 1981 *J. Phys. C: Solid State Phys.* **14** 1919
Carr W J 1966 *Encyclopedia of Physics* vol XVIII/2, ed. H P J Wijn (Berlin: Springer) p 274
Cullen J and Callen E 1984 *Phys. Rev.* B **30** 181
—— 1985 *Physica* B **130** 289
Fisher M E 1974 *Rev. Mod. Phys.* **46** 597
Fontanari J F and Theumann W K 1986 *Phys. Rev.* B **33** 3530
Hathaway K B and Prinz G A 1981 *Phys. Rev. Lett.* **47** 1761
Mukamel D, Fisher M E and Domany E 1976 *Phys. Rev. Lett.* **37** 565
Potts R B 1952 *Proc. Camb. Phil. Soc.* **48** 106
Purwins H G, Walker E, Barbara B, Rossignol M F and Bak P 1974 *J. Phys. C: Solid State Phys.* **7** 3573
Wilson K G and Kogut J 1974 *Phys. Rep.* C **12** 75
Wu F Y 1982 *Rev. Mod. Phys.* **54** 235