J. Phys.: Condens. Matter 5 (1993) 7319–7323. Printed in the UK

Low-temperature expansion for a first-order surface transition

Carla Buzano and Alessandro Pelizzola
Dipartimento di Fisica and Unitá INFM, Politecnico di Torino, I-10129 Torino, Italy

Received 18 June 1993

Abstract. The question concerning the possibility of a first-order surface transition in a semi-infinite Blume–Capel model is addressed by means of low temperature expansions. It is found that such a transition can exist, according to mean field and cluster variation approximations, and in contrast to results from renormalization group approximations.

The semi-infinite spin-1 Blume–Capel model has recently been introduced to describe the surface critical behaviour of magnetic systems [1] and ^{3}He–^{4}He mixtures [2]. The phase diagram of this model has been investigated by means of some well-known methods, namely mean-field approximation (MFA) [1–3], real space renormalization group [4,5] (RG) and the cluster variation method (CVM) [6]. All these methods agree, showing that the model can exhibit three different phases: a completely 'disordered' phase (D) (this phase is called disordered since the magnetic order parameter vanishes, but nevertheless it corresponds to a well-defined ground state, with all spins equal to zero), a completely ordered phase (O) and a partially ordered phase (S), in which order is localized on the surface of the lattice. Only very recently has it been recognized [3] that, at least at the mean field level and for certain values of the model parameters, two different O phases can be found, with different degrees of order at the surface.

Accordingly, different species of phase transitions are found. Lowering the temperature, the model can either order as a whole, passing from the D to the O phase, and the transition is said to be *ordinary*; or it can undergo two different transitions, a *surface* transition from the D to the S phase and then, at a lower temperature, an *extraordinary* transition from the S to the O phase. In the limiting case between these two, the transition is said to be *special*.

In the MFA phase diagram [1] all these transitions can be either second or first order, depending on the model parameters (only the transition between the two O phases considered in [3] is always first order), and this is confirmed by the CVM analysis [6]. On the other hand, the RG scheme developed in [4] (but not the one in [5]) excludes the possibility of extraordinary or surface first-order transitions at finite (i.e. non-zero) temperatures. It is then legitimate to ask whether such transitions do really occur or whether they are only features introduced by some particular approximation.

In the present paper we have addressed this question by means of low-temperature expansions. By using a technique similar to that outlined in [7] in the context of the Pirogov–Sinai theory (although nothing is rigorous for semi-infinite systems) we show that a surface first-order phase transition can be found at low, but non-zero, temperature, and this also implies the existence of an extraordinary first-order transition.

0953-8984/93/407319+05$07.50

Our method consists in expanding the free energies of the S and D phases taking into account only a few excitations over the corresponding ground states. The phase boundary (a first-order transition line) is then determined by comparison of these free energies.

Let us consider the Blume–Capel model on a semi-infinite lattice with a free surface, which is described by the following Hamiltonian:

$$-\beta H = J_s \sum_{\langle ij \rangle} S_i S_j - \Delta_s \sum_i S_i^2 + J_b \sum_{\langle kl \rangle} S_k S_l - \Delta_b \sum_k S_k^2 \tag{1}$$

where $S_i = +1, 0, -1$, $\sum_{\langle ij \rangle}$ denotes a sum over all nearest neighbours (NN) with both sites lying on the surface, $\sum_{\langle kl \rangle}$ denotes a sum over the remaining NN, and $\beta = (k_B T)^{-1}$ (with k_B the Boltzmann constant and T the absolute temperature). J_s and J_b (both positive, since we limit ourselves to the ferromagnetic case) are reduced surface and bulk exchange interactions, while Δ_s and Δ_b are reduced surface and bulk anisotropy, respectively.

In the following we will treat the case $J_b = J_s = J$, $D = \Delta_b/\Delta_s > \frac{3}{2}$ on a simple cubic lattice with a (100) free surface. In such a case (see e.g. [3]) the ground state is O for $\Delta_b < 3J$, S for $3J < \Delta_b < 2DJ$ and D for $\Delta_b > 2DJ$ and, according to mean-field theory, in the $(\Delta_b/6J, T)$ phase diagram, first-order extraordinary and surface transition lines start from $(\frac{1}{2}, 0)$ and $(D/3, 0)$ respectively. Let us now concentrate on the surface transition and develop low-temperature expansions for the surface contributions $f_s^{(S)}$ and $f_s^{(D)}$ to the free energies of the S and D phases.

To begin with, let us consider the S phase, which is characterized by $S_i = +1$ (or, equivalently, -1) for all surface sites, and $S_k = 0$ for all bulk sites. On a lattice with N surface sites, its reduced ground state energy is

$$E_0^{(S)} = N(-2J + \Delta_s)$$

To determine a low-temperature expansion for $f_s^{(S)}$ up to the fifth order in $x = e^{-J}$ we have evaluated all the excitations with respect to the ground state with energy $\delta E < 6J$. An excitation is regarded as a set of spins which are in a state different from the ground state, and is represented by a graph, obtained by drawing a set of circles containing the values of the changed spins and joining with a line each pair of neighbouring spins. We then have surface, bulk and mixed excitations, depending on which spins are changed. To each excitation g (see table 1 for some examples) we have assigned a multiplicity $M(g)$, which is the number of embeddings of the corresponding graph in the lattice under consideration, and a Boltzmann weighting $e^{-\delta E(g)}$.

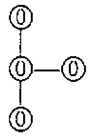
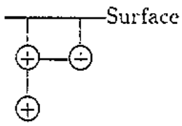
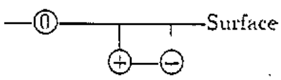
We can thus write the partition function in the form

$$Z^{(S)} = e^{-E_0^{(S)}} \sum_g M(g) e^{-\delta E(g)} \tag{2}$$

which, up to the fifth order in x, reads (for a lattice of L layers, each of N sites)

$$\begin{aligned} Z^{(S)}(N, L) = 2w^{-N}\Big\{1 + N\Big[&(w + y)x^2 + 2(w^2 + (L-2)y + y^2)x^3 \\ &+ \Big([(N-5)/2]w^2 + 6w^3 + w^4 + y + [(N-3)/2]y^2 + 6y^3 + y^4 + (N-1)wy\Big)x^4 \\ &+ 2\Big((N-8)w^3 + 9w^4 + 4w^5 + w^6 \\ &+ (NL - 2N + 3L - 8)y^2 + (N-6)y^3 + 9y^4 + 4y^5 + y^6 \\ &+ (N(L-2)+1)wy + (N-2)w^2 y + (N-2)wy^2\Big)x^5\Big]\Big\} \end{aligned} \tag{3}$$

Table 1. Examples of elementary excitations of the S phase

g	Type	$M(g)$	$\exp[-\delta E(g)]$
	Surface	$4N$	w^4x^5
	Bulk	$4N$	y^3x^5
	Mixed	$2N(N-2)$	wy^2x^5

where $w = e^{\Delta_s - 2J}$ and $y = w^{-D}x^{2\epsilon}$, with $\epsilon = D - 3/2$, are of order unity in the region of the phase diagram that we consider.

Given a partition function $Z(N, L)$, the surface free energy density of the corresponding semi-infinite system is given by [8]

$$f_s = \lim_{N,L\to\infty} \frac{-\ln Z(N,L) - NLf_b}{N} \tag{4}$$

where f_b is the bulk free energy density and is given by

$$f_b = -\lim_{N,L\to\infty} \frac{\ln Z(N,L)}{NL}. \tag{5}$$

We then have, for the surface free energy density of the S phase

$$\begin{aligned} f_s^{(S)} = \; & \Delta_s - 2J - \Big\{(w+y)x^2 + 2(w^2 - 2y + y^2)x^3 \\ & + \Big[w^2\Big(w^2 + 6w - \tfrac{5}{2}\Big) + (1-w)y - \tfrac{3}{2}y^2 + 6y^3 + y^4\Big]x^4 \\ & + 2\Big[w^3(w^3 + 4w^2 + 9w - 8) \\ & + (1-2w)wy - 2(w+4)y^2 - 6y^3 + 9y^4 + 4y^5 + y^6\Big]x^5\Big\}. \end{aligned} \tag{6}$$

In the same way we find

$$\begin{aligned} Z^{(D)}(N,L) = 1 + 2N\Big\{ & w^{-1}x^2 + \Big[2w^{-2} + (L-1)y\Big]x^3 \\ & + \Big[w^{-2}(w^{-2} + 6w^{-1} + N - 5) + w^{-1}y\Big]x^4 \\ & + \Big[2w^{-2}\Big(w^{-4} + 4w^{-3} + 9w^{-2} + 2(N-8)w^{-1} + 1\Big) \\ & + 2(NL - N - 1)w^{-1}y + 4w^{-2}y + (3L-4)y^2\Big]x^5\Big\} \end{aligned} \tag{7}$$

and

$$f_s^{(D)} = -2\Big\{w^{-1}x^2 + (2w^{-2} - y)x^3 + \Big[w^{-2}(w^{-2} + 6w^{-1} - 5) + w^{-1}y\Big]x^4 + \Big[2w^{-2}(w^{-4} + 4w^{-3} + 9w^{-2} - 16w^{-1} + 1) - 2(1 - 2w^{-1})w^{-1}y - 4y^2\Big]x^5\Big\}. \tag{8}$$

The transition line is then readily obtained by numerically solving the equation $f_s^{(S)} = f_s^{(D)}$ for $\Delta_b/6J$ at each temperature, and is reported in figure 1 together with MFA and CVM results, for a choice of values of the model parameters. The transition is first order, as is checked below, and the results of MFA and CVM are qualitatively confirmed (the reentrance predicted by CVM is not seen here). The above results should be particularly reliable for $\epsilon < \frac{1}{12}$ (in order to satisfy $\delta E(g) < 6J$ for all the excitations considered) and for $k_B T/6J < 0.06$, so that the fifth-order contributions are no more than a few percent of the sum of the lower-order terms (excluding the zeroth-order terms, of course, since they are defined up to an additive constant), and these conditions are satisfied in figure 1.

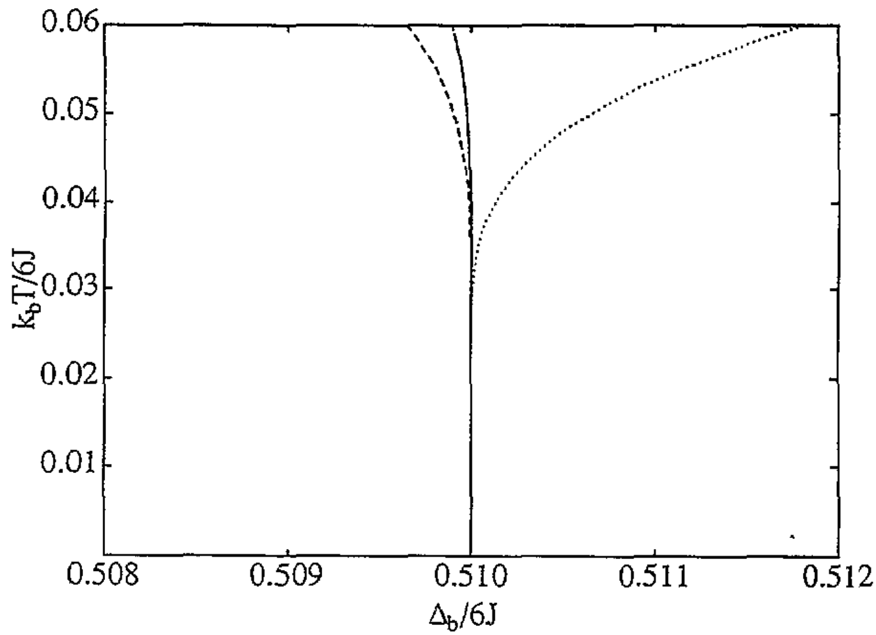


Figure 1. Surface first-order transition lines for $\epsilon = 0.03$ as given by the present method (solid line), MFA (dashed line) and CVM (dotted line).

One can check that the transition is indeed first order by looking at, for example, the surface quadrupolar order parameter

$$q_s = (\partial f_s/\partial \Delta_s).$$

This is the expected value of S_i^2, where S_i is a surface spin, and its ground state values are one for the S phase and zero for the D phase. In the case of figure 1, the jump in q_s at the transition is greater than 0.98 in the range of temperatures considered, which denotes a strong first-order transition.

Implicitly, since the bulk phase diagram is simply the phase diagram of the infinite system, which is also known to undergo a first-order transition, our results show that the Blume–Capel model on a semi-infinite lattice is also capable of exhibiting an extraordinary first-order transition.

Summarizing, we have shown by low-temperature expansions that the surface transition of the semi-infinite Blume–Capel model can be also first order, according to previous results obtained by MFA and CVM, and in contrast with an RG analysis. We believe that the present method is more accurate than the RG scheme proposed in [4], since this kind of low-temperature expansion, even if not rigorous in the presence of a free surface, is particularly well suited for first-order transitions. Furthermore, RG schemes for models with several different phases and rich phase diagrams heavily depend on the choice of the mapping truncation. This can be seen by comparing the results in [4], which exclude the possibility of a surface or extraordinary first-order transition, with those in [5], where, by means of a different RG scheme, such transitions are found. Indeed, only very recently Berker and Netz [9] have succeeded in devising an RG scheme capable of describing the antiquadrupolar and ferrimagnetic phases of the Blume–Emery–Griffiths model.

References

[1] Benyoussef A, Boccara N and Saber M 1986 *J. Phys. C: Solid State Phys.* **19** 1983
[2] Yiang X P and Giri M R 1988 *J. Phys. C: Solid State Phys.* **21** 995
[3] Buzano C and Pelizzola A in preparation
[4] Benyoussef A, Boccara N and El Bouziani M 1986 *Phys. Rev.* B **34** 7775
[5] Peliti L and Leibler S 1984 *J. Physique Lett.* **45** L591
[6] Buzano C and Pelizzola A 1993 *Physica* A **195** 197
[7] Slawny J 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (London: Academic) ch 3
[8] Pandit R, Schick M and Wortis M 1982 *Phys. Rev.* B **26** 5112
[9] Netz R R and Berker A N 1993 *Phys. Rev.* B **47** 15019