LOW–TEMPERATURE EXPANSION FOR A FIRST ORDER SURFACE TRANSITION

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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 contrarily to renormalization group results.
The semi–infinite spin–1 Blume–Capel model has been recently introduced to describe the surface critical behavior of magnetic systems[1] and $^3\text{He}–^4\text{He}$ mixtures[2]. The phase diagram of this model has been investigated by means of some well–known methods, namely mean field approximation[1–3] (MFA), real space renormalization group[4,5] (RG) and cluster variation method[6] (CVM). All these methods agree to show that the model can exhibit three different phases: a completely disordered phase (D), 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 it has been recognized[3] that, at least at the mean field level, 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 one from the D to the S phase and then, at a lower temperature, an extraordinary one from the S to the O phase. In the limiting case between the two above, 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. nonzero) temperatures. It is then legitimate to ask whether such transitions do really occur or they are only features introduced by some particular approximation.

In the present Letter 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 nonzero, temperature, and this also implies the existence of an extraordinary first order transition.
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 energy.

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 neighbors (n.n.) with both sites lying on the surface, $\sum_{\langle kl \rangle}$ denotes a sum over the remaining n.n., and $\beta = (k_B T)^{-1}$ (with $k_B$ Boltzmann constant and $T$ 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 $\Delta_s$ and $\Delta_b$ are reduced surface and bulk anisotropy, respectively.

In the following we will treat the case $J_b = J_s = J, D = \Delta_b/\Delta_s > 3/2$ 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 $(1/2, 0)$ 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 5th order in $x = e^{-J}$ we have enumerated 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 drawing a set of circles containing the
values of the changed spins and joining with a line each pair of neighboring spins. We have then surface, bulk and mixed excitations, depending on which spins are changed. To each excitation \( g \) (see Tab. I 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 weight \( e^{-\delta E(g)} \).

We can thus write the partition function in the form

\[
Z^{(S)} = e^{-E^{(S)}_0} \sum_g M(g)e^{-\delta E(g)},
\]

which, up to the 5th order in \( x \), reads (for a lattice of \( L \) layers, each of \( N \) sites)

\[
Z^{(S)}(N, L) = 2w^{-N} \left\{ 1 + N \left[ (w + y)x^2 + 2(w^2 + (L - 2)y + y^2)x^3 \\
+ \left( \frac{N - 5}{2} w^2 + 6w^3 + w^4 + y + \frac{N - 3}{2} y^2 + 6y^3 + y^4 + (N - 1)wy \right) x^4 \\
+ 2 \left( (N - 8)w^3 + 9w^4 + 4w^5 + w^6 \\
+ (NL - 2N + 3L - 8)y^2 + (N - 6)y^3 + 9y^4 + 4y^5 + y^6 \\
+ (N(L - 2) + 1)wy + (N - 2)w^2y + (N - 2)wy^2 \right) x^5 \right] \right\},
\]

where \( w = e^{\Delta_s - 2J} \), \( y = w^{-D} x^{2\epsilon} \) and \( \epsilon = D - 3/2 \).

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

\[
f_s = \lim_{N,L \to \infty} -\frac{\ln Z(N, L) - NL f_b}{N},
\]

where \( f_b \) is the bulk free energy density and is given by

\[
f_b = -\lim_{N,L \to \infty} \frac{\ln Z(N, L)}{NL}.
\]
We then have, for the surface free energy density of the S phase:

\[
f_s^{(S)} = \Delta_s - 2J - \left\{(w + y)x^2 + 2(w^2 - 2y + y^2)x^3 \right. \\
+ \left[w^2 \left(w^2 + 6w - \frac{5}{2}\right) + (1 - w)y - \frac{3}{2}y^2 + 6y^3 + y^4 \right]x^4 \\
+ 2 \left[w^3(w^3 + 4w^2 + 9w - 8) \\
+ (1 - 2w)wy - 2(w + 4)y^2 - 6y^3 + 9y^4 + 4y^5 + y^6 \right]x^5 \right\}.
\]

(6)

In the same way we find

\[
Z^{(D)}(N, L) = \\
1 + 2N \left\{ w^{-1}x^2 + \left[2w^{-2} + (L - 1)y \right]x^3 \\
+ \left[w^{-2}(w^{-2} + 6w^{-1} + N - 5) + w^{-1}y \right]x^4 \\
+ \left[2w^{-2}(w^{-4} + 4w^{-3} + 9w^{-2} - 2(N - 8)w^{-1} + 1) \\
+ 2(NL - N - 1)w^{-1}y + 4w^{-2}y + (3L - 4)y^2 \right]x^5 \right\}
\]

(7)

and

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

(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 Fig. 1 together with MFA and CVM results, for a choice of values of the model parameters. The transition is first order, as can be checked by looking at derivatives of the free energies, 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 \(\epsilon < 1/12\) (in order to satisfy \(\delta E(g) < 6J\) for all the excitations considered) and for \(k_BT/6J < 0.06\),
so that the 5th order contributions are no more than a few percent of the sum of the lower order terms (excluding the 0th order ones, of course, since they are defined up to an additive constant), and these conditions are satisfied in Fig. 1.

Implicitly, since the bulk phase diagram is simply the phase diagram of the infinite system, which is known to undergo also 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 a 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, as 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 [9] Berker and Netz have succeeded in devising a RG scheme capable of describing the antiquadrupolar and ferrimagnetic phases of the Blume–Emery–Griffiths model.
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Figure Caption

Fig. 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).
Table I. Examples of elementary excitations of the S phase

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