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Mean-field-like approximations to critical behaviour at surfaces

H A Ceccatto

Instituto de Física Rosario—CONICET/UNR, Av. Pellegrini 250, 2000 Rosario, Republica Argentina

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Abstract. Improved mean-field-like approximations to critical behaviour at surfaces are considered. By using the high-temperature expansion of the 2D Ising model susceptibility, good estimates for critical values of the 3D semi-infinite Ising model are obtained. As an example, the critical surface coupling enhancement is found to be $\Delta_C = 0.44$, which must be compared with the standard mean-field approximation value $\Delta_C^{MF} = 0.25$ and the recent Monte Carlo result $\Delta_C^{MC} = 0.50 \pm 0.03$.

Critical phenomena associated with free magnetic surfaces have been investigated for many years (for a review see Binder (1983)). From a theoretical point of view, the standard example is the semi-infinite Ising model with modified exchange on the free surface (Mills 1971). This system can be viewed as a d-dimensional Ising film of N layers ($N \to \infty$), in which the spins in the free surface interact among one another with an exchange parameter K_S ($= J_S/kT$) which is different from the bulk exchange K ($= J/kT$). Usually it is assumed that $K_S = (1+\Delta)K$, where Δ is known as the surface coupling enhancement.

For $d > 2$ this simple system has, in addition to the bulk transition, surface para-ferromagnetic transitions and a simultaneous surface-bulk transition for suitable enhanced K_S. In the surface ferromagnetic phase the magnetisation goes monotonically to zero when one penetrates into the bulk. This phase becomes possible for K_S greater than a critical value $K_{SB}^C = (1+\Delta_C)K^C$ at which the simultaneous (special) surface-bulk transition takes place. Here Δ_C, the critical enhancement, is a still unknown (exactly) finite value and K^C is the bulk critical coupling.

The classical mean-field approximation (MFA) gives for the simple cubic lattice $\Delta_C = \frac{1}{4}$; more sophisticated theories have provided different values for Δ_C (for an account of these values see Tsallis and Sarmento (1985)), which are to be compared with the more reliable series ($\Delta_C^S = 0.6 \pm 0.1$ (Binder and Hohenberg 1974)) and Monte Carlo ($\Delta_C^{MC} = 0.50 \pm 0.03$ (Binder and Landau 1984)) results.

Recently Plascak (1984) has improved on the MF values through a variational procedure, which essentially treats in an exact fashion parallel spin chains on each layer. Interactions between chains are simulated through external fields, which are considered as variational parameters. They are determined by minimising the variational free energy

$$F_0[\mathscr{H}_0] + \langle \mathscr{H} - \mathscr{H}_0 \rangle_0 \geqslant F[\mathscr{H}] \tag{1}$$

where $\mathscr{H}$ is the model Hamiltonian and $\mathscr{H}_0$ is the Hamiltonian of the (uncoupled) spin chains in external fields. Thermal averages $\langle\ \rangle_0$ are taken with respect to $\exp(-\beta\mathscr{H}_0)$. This procedure leads to self-consistent values for the external fields as in the variational formulation of the standard MF theory. Of course, it also provides the classical MF values for critical exponents.

Here we discuss different MF-like approaches to critical behaviour at surfaces, closely related to Plascak's work but which greatly improve on its results, as can be seen in figure 2.

Firstly we consider for $d=3$ a somewhat obvious generalisation of the procedure described above by taking as a trial Hamiltonian

$$\mathscr{H}_0=\sum_n \mathscr{H}_n^{2\mathrm{D}}+\sum_{n,x} \gamma_n S_x^n$$

where $\mathscr{H}_n^{2\mathrm{D}}$ is the 2D Ising Hamiltonian defined by the spins interacting on the nth layer. The self-consistent fields γ_n simulate the interaction between spins on adjacent layers. They can also be considered as variational parameters and be determined by minimising (1). Thus, we obtain

$$\gamma_n=K(m_{n+1}+m_{n-1}) \tag{2}$$

where m_n is the magnetisation per site on the nth layer and $m_{n-1}=0$ for $n=1$.

At first sight it appears difficult to handle the effective 2D Ising systems coupled to external γ_n fields. In fact, for continuous phase transitions and near the critical points we can consider γ_n to be infinitesimal. Then the magnetisations are

$$m_n \simeq \chi_n(\gamma_n+H_n). \tag{3}$$

In this equation $\chi_n=\chi(K_n)$ ($K_n=K$, $n\geq 2$, $K_1=K_{\mathrm{S}}$) is the susceptibility per site of a 2D Ising model in zero field and we have introduced infinitesimal polarising fields H_n.

By proposing as usual a magnetisation profile

$$m_n=m+\delta\exp[-q(n-1)] \qquad (q\geq 0) \tag{4}$$

when $n\to\infty$ from equations (2)-(3) we get the bulk magnetisation:

$$m=\chi H/D, \qquad D=1-2K\chi(K). \tag{5a}$$

The same equations lead, for finite n, to

$$\mathrm{e}^q=[1+(1-4K^2\chi^2)^{1/2}]/2K\chi$$

and

$$\delta=\frac{\mathrm{e}^q\chi(K_{\mathrm{S}})}{D_{\mathrm{S}}}H_{\mathrm{S}}+\frac{\mathrm{e}^q[D\chi(K_{\mathrm{S}})+K\chi(K)\chi(K_{\mathrm{S}})-\chi(K)]}{DD_{\mathrm{S}}}H$$

where

$$D_{\mathrm{S}}=\mathrm{e}^q-K\chi(K_{\mathrm{S}}). \tag{5b}$$

The bulk and surface-bulk critical couplings can now be determined from $D(K^{\mathrm{C}})=0$ and $D_{\mathrm{S}}(K^{\mathrm{C}}, K_{\mathrm{SB}}^{\mathrm{C}})=0$. To evaluate these equations numerically we use the high-temperature series expansion of χ (Domb 1974). Thus, we get† $K^{\mathrm{C}}=0.189$, $K_{\mathrm{SB}}^{\mathrm{C}}=0.272$ and then a critical surface coupling enhancement $\Delta_{\mathrm{C}}=0.44$. This value for Δ_{C}

† We have obtained these results with the first 15 terms of the χ expansion and have checked that higher-order terms do not modify them.

is quite satisfactory; it approaches the Monte Carlo one ($\Delta_{\mathrm{C}}^{\mathrm{MC}}=0.50\pm0.03$) more than any other theory we are aware of. In figure 2 we compare these values (curve A) with those corresponding to the MFA and Plascak's work (curves MF and P respectively).

To improve the above results we must introduce correlations between sites placed at different layers. This can be done by considering, as in the Bethe approximation (Domb 1960), spin clusters such as those shown in figure 1.

In this case, the magnetisations of the central (c) and boundary (b) sites on the nth layer are

$$m_n^{\mathrm{c}}=\tanh K_n[\alpha_{n+1}+\alpha_{n-1}+2(d-1)\alpha_n], \tag{6a}$$

$$m_n^{\mathrm{b}}=\tanh^2 K_n(\alpha_{n+1}+\alpha_{n-1})+[1+(2d-3)\tanh^2 K_n]\alpha_n, \tag{6b}$$

where α_n is the (infinitesimal) self-consistent field felt by the boundary site on the nth layer near the bulk transition temperature. As in equation (2) we can consider this field as created by the nearest-neighbour site magnetisations:

$$\alpha_n=K(m_{n+1}+m_{n-1})+(2d-3)K_n m_n. \tag{6c}$$

In (6) we have called, as above, $K_1=K_{\mathrm{S}}$, $K_n=K$ $(n\geqslant 2)$. For $n=1$ we must take $m_{n-1}=\alpha_{n-1}=0$.

Taking into account (4), the consistency conditions

$$m_n^{\mathrm{c}}=m_n^{\mathrm{b}}=m_n, \qquad \forall n, \tag{7}$$

lead, for $n\to\infty$, to

$$\tanh K^{\mathrm{C}}=1/(2d-1) \tag{8a}$$

which is the known Bethe approximation result for the bulk critical coupling. When $n=1$ we get for $K_{\mathrm{SB}}^{\mathrm{C}}$ the equation

$$K^{\mathrm{C}}+2(d-1)\tanh K_{\mathrm{SB}}^{\mathrm{C}}[K^{\mathrm{C}}+(2d-3)K_{\mathrm{SB}}^{\mathrm{C}}]=K^{\mathrm{C}}\tanh K_{\mathrm{SB}}^{\mathrm{C}}$$
$$+[1+(2d-3)\tanh^2 K_{\mathrm{SB}}^{\mathrm{C}}][K^{\mathrm{C}}+(2d-3)K_{\mathrm{SB}}^{\mathrm{C}}]. \tag{8b}$$

For $d=3$ numerical evaluations of (8) give $K^{\mathrm{C}}=0.203$, $K_{\mathrm{SB}}^{\mathrm{C}}=0.274$ and consequently, $\Delta_{\mathrm{C}}=0.35$. As expected, this approximation leads to a K^{C} better than that previously obtained from (5). Note also that, in spite of the worse Δ_{C} value, $K_{\mathrm{SB}}^{\mathrm{C}}$ has been a little improved (see figure 2, curve B).

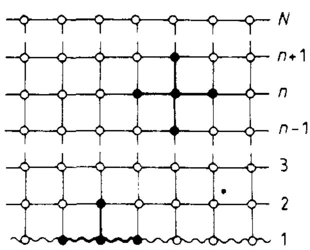

Figure 1. Two-dimensional cross section of the clusters considered in the text (full circles). Open circles are spins fixed at their mean value. Full lines indicate exchange coupling $K(=J/kT)$ while wavy lines indicate surface exchange coupling K_{S} $(=J_{\mathrm{S}}/kT)$.

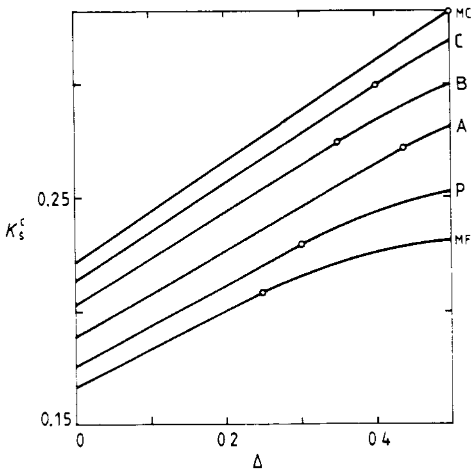

Figure 2. Surface critical coupling K_S^C as a function of the enhancement Δ. We have adopted this way of representing the phase diagram to show, in a single figure, the relevant values $K^C = K_S^C(\Delta = 0)$, $K_{SB}^C = K_S^C(\Delta = \Delta_C)$ and Δ_C. Open circles have coordinates (Δ_C, K_{SB}^C) as given for the different approximations. Curve MF: mean-field approximation; curve P: Plascak's work; curves A, B, C: present work, equations (5), (8) and (9) respectively. Monte Carlo (MC) results (Binder and Landau 1984) are also shown for comparison.

Finally, we can combine the two previous approximations in such a way as to have an exact treatment of interactions on each layer (as in the first approach) and, simultaneously, to incorporate correlations between sites on adjacent surfaces (as in the second one). To do this we replace the Bethe consistency condition (7) by $m_n^{\text{layer}} = m_n^c = m_n$, i.e., we enforce the central site of the cluster to have the same magnetisation as an arbitrary site on the fully coupled layer. Thus the critical values verify

$$\chi(K^C) = d(2d-1)\tanh K^C \tag{9a}$$

and

$$(2d-1)K^C \tanh K^C + 2(d-1)\tanh K_{SB}^C[K^C + (2d-3)K_{SB}^C] = K^C\chi(K_{SB}^C). \tag{9b}$$

From these equations we get $K^C = 0.213$, $K_{SB}^C = 0.299$ and $\Delta_C = 0.40$. Also in this case a slightly worse value for Δ_C is obtained. However, we have in fact achieved a considerable improvement on the surface-bulk critical value and the bulk critical coupling (nearly 4% off the most reliable value $K^C = 0.2217$) (see figure 2, curve C).

In conclusion, we have shown that simple MF-like techniques plus available results from 2D systems (χ expansion) lead to good estimates for critical values in 3D systems with a free surface.

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