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1987 J. Phys. A: Math. Gen. 20 6143

(http://iopscience.iop.org/0305-4470/20/17/048)

J. Phys. A: Math. Gen. 20 (1987) 6143-6146. Printed in the UK

COMMENT

Mean-field renormalisation group study of the semi-infinite Potts model

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Received 21 April 1987

Abstract. The MFRG method is used to study the critical behaviour of the semi-infinite three-dimensional q-state Potts model. Estimates of Δ_c, the critical enhancement at the special transition, and the phase diagram are obtained for different values of q and compared with results from other techniques.

Surface effects in phase transitions have received a great deal of attention in the past few years (see [1] for a review). The critical behaviour of the semi-infinite Ising model seems to be reasonably well understood and so are models with a continuous symmetry (see [2] for a recent study). The q-state Potts model is an interesting generalisation of the Ising ($q=2$) case which deserves special attention since it has some new features, namely the alteration of the order of the phase transition for $q=q_c(d)$. This offers the possibility for a semi-infinite system to have a continuous surface transition whereas the bulk (ordinary) transition is discontinuous [3]. This expectation appears to have been confirmed experimentally [4].

In the present work we use the MFRG technique to obtain the phase diagram of the Potts ferromagnet in a simple cubic lattice with a free surface, generalising our recent study [5] on the semi-infinite Ising ferromagnet.

Two clusters, I and II, with respectively 2 and 4 spins are considered (figure 1); we write their Hamiltonians:

$$\mathscr{H}_{\mathrm{I}} = -J'_{\mathrm{B}} \sum_{k=1}^{q} P_1^k P_2^k - h'_1 \pi_1^1 - h'_2 \pi_2^1 \tag{1a}$$

and

$$\mathscr{H}_{\mathrm{II}} = -\sum_{k=1}^{q} (J_s P_1^k P_2^k + J_{\mathrm{B}}(P_2^k P_3^k + P_3^k P_4^k + P_4^k P_1^k)) - h_1(\pi_1^1 + \pi_2^1) - h_3(\pi_3^1 + \pi_4^1) \tag{1b}$$

(where P^k is the projector onto the kth Potts state, $\pi^k \equiv P^k - 1/q$). h'_1, h'_2, h_1, h_3 are effective fields representing the interaction of spins in a cluster with their neighbours outside the cluster. Near the surface transition line we let $h'_1 = 4J'_s C'_s$, $h'_2(=5J'_{\mathrm{B}}C'_{\mathrm{B}})=0$,

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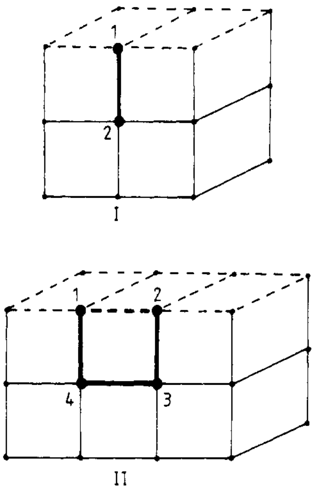

Figure 1. Clusters I and II. $J_s'(J_s)$ (broken lines), $J_B'(J_B)$ (full lines).

$h_1 = 3J_sC_s$ and $h_3(=4J_BC_B) = 0$ and assume that C_s' and C_s scale like the corresponding surface magnetisations

$$\frac{\langle \pi_1^1 \rangle_I}{\frac{1}{2}\langle \pi_1^1 + \pi_2^1 \rangle_{II}} = \frac{C_s'}{C_s} \qquad (2)$$

where $\langle \pi_1^1 \rangle_I$ $(\frac{1}{2}\langle \pi_1^1 + \pi_2^1 \rangle_{II})$ denotes the average surface magnetisation in cluster I (II). Linearising with respect to effective fields C_s and C_s', equation (2) leads, after some lengthy algebra, to the recursion relation

$$\begin{aligned} K_s[&4\exp(K_s+3K_B)+6(q-2)\exp(2K_B)+12(q-1)\exp(K_s+K_B)\\ &+2(q-2)(q^2-3q+3)+6(q-2)^2\exp(K_B)\\ &+4(q-1)(q-2)\exp(K_s)]\\ &\times\{\exp(K_s+3K_B)+3(q-1)[\exp(2K_B)\exp(K_s+K_B)]\\ &+(q-1)(q^2-3q+3)+3(q-1)(q-2)\exp(K_B)\\ &+(q-1)(q-2)\exp(K_s)\}^{-1}=\tfrac{8}{3}K_s' \end{aligned} \qquad (3)$$

with $K_s = J_s/KT$, $K_B = J_B/KT$. The surface transition line is obtained from the fixed point equation (derived from (3) with $K_s = K_s'$, $K_B = K_B'$).

To calculate the bulk critical temperature we consider clusters I and II away from the surface with $J_B = J_s$, $J_B' = J_s'$, $h_1' = h_2' = 5J_B'C_B'$, $h_1 = h_3 = 4J_BC_B$ and proceed as above, with C_B and C_B' replacing C_s and C_s' and the bulk magnetisation in the place of the surface magnetisation. One gets, in this case

$$\begin{aligned} K_B\{&8\exp(4K_B)+[12(q-2)+8(2q-3)]\exp(2K_B)+2(q-2)(q^2-4q+6)\\ &+[8(q-2)(q-3)+4(q-2)^2]\exp(K_B)\}\\ &\times[\exp(4K_B)+6(q-1)\exp(2K_B)+(q-1)(q^2-3q+3)\\ &+4(q-2)(q-1)\exp(K_B)]^{-1}\\ =\tfrac{5}{2}&K_B'[2\exp(K_B')+q-2][\exp(K_B')+q-1]^{-1} \end{aligned} \qquad (4)$$

where K_B^C is the non-trivial fixed point solution of (4). If in (3) we write $K_s = K_B(1+\Delta)$, and set $K_B = K_B^C$, we obtain Δ_c, the critical enhancement at the special transition.

Phase diagrams obtained from (3) and (4) are represented in figure 2 for some values of q. Expressions (2)-(4) implicitly assume continuous transitions. However, though the MFRG technique was originally designed for second-order phase transitions and is not able to answer questions about the order of the transition, it still gives a reliable prediction for the transition temperature in situations where the transition is known to be first order [6-8]. We therefore expect the overall behaviour depicted in figure 2 to be correct, namely in the cases $q = 3$ and $q = 4$ where one expects a continuous surface transition and a weakly first-order bulk transition. In table 1 we show some values of Δ_c as well as the corresponding exponent ϕ which measures the curvature of the surface transition line at Δ_c: $(T_c(\Delta) - T_c)/T_c \sim (\Delta - \Delta_c)^{1/\phi}$ when $\Delta \to \Delta_c^+$. Whenever the surface transition is second order, ϕ describes the crossover from multicritical behaviour at $\Delta = \Delta_c$ to two-dimensional critical behaviour.

Table 1.

q	Δ_c	ϕ
1	0.73	0.81
2	0.64	0.83
3	0.59	0.84
4	0.55	0.845

Our results are in qualitative agreement with Tsallis and Sarmento [9] who looked at the same system using MKRG in a hierarchical lattice. Their technique enabled them to study RG fixed points and flows but is not capable of tracing first-order transitions either. Our method is a lot simpler to apply, through more limited in scope, and it gives a better prediction for $\Delta_c(q = 2)$ as compared to Monte Carlo [10] (we are not aware of MC or other numerical studies for general q). When $q \to 0$ our results are not consistent with $\Delta_c \sim q^{-1/2}$ predicted by Tsallis and Sarmento.

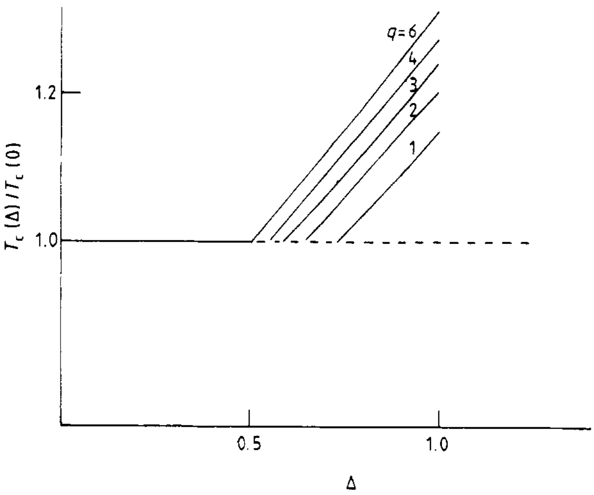

Figure 2. Phase diagram for $q = 1, 2, 3, 4, 6$.

MAS would like to thank R Stinchcombe for helpful discussions. A sabbatical grant from INIC (Portugal) is also gratefully acknowledged.

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