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LETTER TO THE EDITOR

A renormalisation group analysis of the semi-infinite Potts model

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Abstract. We discuss the ordinary transition of the semi-infinite q-state Potts model within the Migdal–Kadanoff renormalisation group scheme. Approximate surface free energies are calculated in dimension $D = 2$. In addition, we consider the effect of symmetry breaking surface fields. Our scheme predicts that only one such field is relevant.

We consider the q-state Potts model for a semi-infinite hypercubic lattice in D dimensions. On each lattice site i, we place a Potts spin variable $\sigma_i = 1, 2, \ldots, q$. The set of all surface sites is denoted by Λ_s. The Hamiltonian of this model is given by

$$-\beta\mathscr{H} = \sum_{\langle ij\rangle} K_{ij}\delta(\sigma_i, \sigma_j), \tag{1a}$$

$$K_{ij} = \begin{cases} K_s & i, j \in \Lambda_s, \\ K & \text{otherwise.} \end{cases} \tag{1b}$$

$\langle ij\rangle$ indicates a sum over nearest neighbours, and $\delta(\sigma_i, \sigma_j)$ is the Kronecker symbol which is 1 iff $\sigma_i = \sigma_j$ and 0 otherwise.

For $q = 2$, this model is equivalent to the semi-infinite Ising model. In this case, various methods have been used to calculate both the phase diagram as well as thermodynamic functions and scaling indices (e.g. Au Yang 1973, Binder and Hohenberg 1974, Burkhardt and Eisenriegler 1977). Recently, we have shown that the simple Migdal–Kadanoff renormalisation group (MKRG) approach (Migdal 1975, Kadanoff 1976) is also adequate (Lipowsky and Wagner 1981). Similar approaches have been used independently by Nagai and Toyonaga (1981) and by Parga and van Himbergen (1981).

For $q \geq 3$, we naively expect that the phase diagram in the (K, K_s) plane is similar to the corresponding phase diagram of the Ising model: for $D = 2$, the system should undergo an ordinary transition, while for $D = 3$, there should be a surface, an ordinary, a surface-bulk or special, and an extraordinary transition (for the terminology in the Ising case, see e.g. Burkhardt and Eisenriegler (1977)). For $q \geq 3$, however, these phase transitions may be either continuous or discontinuous. For instance, for $q = 3$, 4 and $D = 3$ we expect that the surface transition is continuous while the other transitions are discontinuous. In addition, a new type of phase transition occurs for large q (Lipowsky 1981 a,b). At this new transition, the surface order parameter jumps while the bulk order parameter varies smoothly.

In this Letter, we apply the MKRG scheme as described in Lipowsky and Wagner (1981) for the semi-infinite Ising model to model (1). It is well known that this scheme yields a continuous bulk transition for all finite q and $D>1$. A discontinuous bulk transition is obtained only in the many-component limit $q\to\infty$ (Berker and Ostlund 1979). However, it is known exactly that this bulk transition is discontinuous for $q>4$ in $D=2$ (Baxter 1973). In addition, both recent field theoretic RG calculations (Aharony and Phytte 1981) and position-space RG calculations for the dilute Potts model (e.g. Nienhuis *et al* 1981) indicate that the three-dimensional bulk transition is discontinuous for $q\geqslant 3$. Therefore, we will mainly discuss the case $D=2$ and $q=3$, 4 where the MKRG scheme yields the correct nature of the bulk transition. The MKRG analysis for the many-component limit $q\to\infty$ of model (1) is discussed elsewhere (Lipowsky 1981a).

Within the MKRG scheme, we obtain the following differential recursion relations:

$$\mathrm{d}K/\mathrm{d}l=(D-1)K-B_q(K)/q, \tag{2a}$$

$$\mathrm{d}K_s/\mathrm{d}l=\tfrac{1}{2}K+(D-2)K_s-B_q(K_s)/q, \tag{2b}$$

$$B_q(x)=[\mathrm{e}^x+(1-q)\mathrm{e}^{-x}+q-2]\ln[1+q/(\mathrm{e}^x-1)]. \tag{2c}$$

The bulk recursion relation (2a) yields the exact critical coupling $K^c=\ln(1+\sqrt{q})$ (Stephen 1976). This is due to the fact that the differential MKRG transformation and the duality transformation commute. The phase diagram obtained from (2) for $D=2$ and $q=3, 4$ is similar to the phase diagram of the semi-infinite Ising model as expected. There is only one non-trivial fixed point (K^c, K_s^c) on which the line $K=K^c$ associated with the ordinary transition is mapped under the RG. At this fixed point, the linearised recursion relations lead to one relevant and one irrelevant temperature-like perturbation corresponding to $\delta K:=K-K^c$ and $\delta K_s:=K_s-K_s^c$ respectively.

For $D=2$ and $q\geqslant q^*=41$, (2) yields an additional multicritical fixed point with two relevant temperature-like perturbations. This fixed point is rather unexpected. However, it is related to a genuine structure of the phase diagram of model (1). A mean field analysis shows that there is a new type of phase transition for large q in the low-temperature regime $K>K^c$ (Lipowsky 1981b). At this new transition, the surface order parameter jumps while the bulk order parameter varies smoothly. In the extreme case $q\to\infty$, this leads to a low-temperature phase where the surface spins are completely uncorrelated (Lipowsky 1981a).

Next, we calculate approximate bulk and surface free energies within the MKRG approach. The approximate bulk free energy $f_B(K)$ is given by the trajectory integral (cf Lipowsky and Wagner 1981)

$$f_B(K)=D\int_0^\infty \mathrm{d}l\ \mathrm{e}^{-Dl}g_q[\tilde{K}(l,K)] \tag{3a}$$

where $\tilde{K}(l,K)$ is the solution of (2a) with the initial condition $\tilde{K}(0,K)=K$ and

$$g_q(x)=(\omega_1\ln\omega_1-\omega_2\ln\omega_2)/q, \qquad \omega_1=\mathrm{e}^x+q-1, \qquad \omega_2=\mathrm{e}^x-1. \tag{3b}$$

$\omega_{1/2}$ are the eigenvalues of the transfer matrix for the one-dimensional bulk problem. In (3a), we have used the boundary condition

$$\lim_{l\to\infty}\mathrm{e}^{-Dl}f_B(l)=0.$$

From (3a), one obtains

$$f_B(K) \to \begin{cases} \ln q + DK/q & K \to 0, \\ DK & K \to \infty, \end{cases} \tag{4}$$

which is the exact asymptotic behaviour for all q and D. In the two-dimensional Ising model ($q=2$), we compared the approximate $f_B(K)$ obtained via (3a) with the exact $f_B(K)$ which is known for all K. In this case, the relative error is less than 3% over the whole temperature region (Lipowsky and Wagner 1981). The maximum of the relative error occurs at $K=K^c$. For $q \geq 3$ and $D=2$, only $f_B(K=K^c)$ is known exactly (Baxter 1973). From (3) and (2a), we obtain the approximate value

$$f_B(K^c) = \tfrac{1}{2}\ln q + [(1+\sqrt{q})/\sqrt{q}]\ln(1+\sqrt{q}) \tag{5a}$$

in $D=2$. For $q=3$ and 4, (5a) yields $f_B(K^c)=2.13$ and 2.34 which should be compared with the exact values $f_B(K^c)=2.07$ and 2.26 respectively. Thus, the relative error is less than 4%. From (3) and (2a), we may also obtain an approximate bulk energy $\varepsilon_B := -\mathrm{d}f_B/\mathrm{d}K$ at the transition temperature:

$$\varepsilon_B(K^c) = -(1+1/\sqrt{q}). \tag{5b}$$

For $q=2$, (5b) is exact (cf e.g. McCoy and Wu 1973).

The approximate surface free energy $f_s(K, K_s)$ is given by the trajectory integral

$$f_s(K, K_s) = \int_0^\infty \mathrm{d}l\, \mathrm{e}^{-(D-1)l} G[K(l,K), K_s(l,K,K_s)] + C_s(K,K_s) \tag{6a}$$

with

$$G(K,K_s) = (D-1)[g_q(K_s) - g_q(K)] + \tfrac{1}{2}[f_B(K) - g_q(K)] \tag{6b}$$

where $f_B(K)$ and $g_q(x)$ are given by (3a) and (3b) respectively. We choose the boundary condition

$$C_s(K,K_s) := \lim_{l\to\infty} \mathrm{e}^{-(D-1)l} f_s(l)$$
$$= \begin{cases} 0 & K<K^c, \\ -\tfrac{1}{2}DK + \tfrac{1}{2}D/(D-1) & K>K^c, \end{cases} \tag{6c}$$

as in the Ising case (Lipowsky and Wagner 1981).

In the low- and high-temperature limits one finds from (6a)

$$f_s(K,K_s) \to \begin{cases} [(D-1)(-K+K_s) - K/2]/q & K, K_s \to 0, \\ (D-1)(-K+K_s) - K/2 & K, Ks \to \infty, \end{cases}$$

which is the exact asymptotic behaviour for all q and D. For intermediate coupling constants, we may calculate the trajectory integral (6a) numerically. In figure 1(a), we depict the surface free energies f_s for $q=3$ along the temperature trajectories $(K, K_s=\gamma K)$ with $\gamma=\tfrac{1}{2}$, 1, $\tfrac{3}{2}$ and 2. In figure 1(b), we compare the surface free energies f_s with $\gamma=1$ for $q=2$, 4 and 10. The surface free energy $\bar{f}_s$ of the two-dimensional Ising model with $\gamma=1$ is obtained via

$$\bar{f}_s(J, J_s=J) = f_s(K=2J, K_s=2J_s; q=2) + \tfrac{3}{2}J - J_s. \tag{7}$$

The function $\bar{f}_s$ is known exactly (McCoy and Wu 1973). It has been discussed previously within the MKRG scheme (Lipowsky and Wagner 1981). Note that the

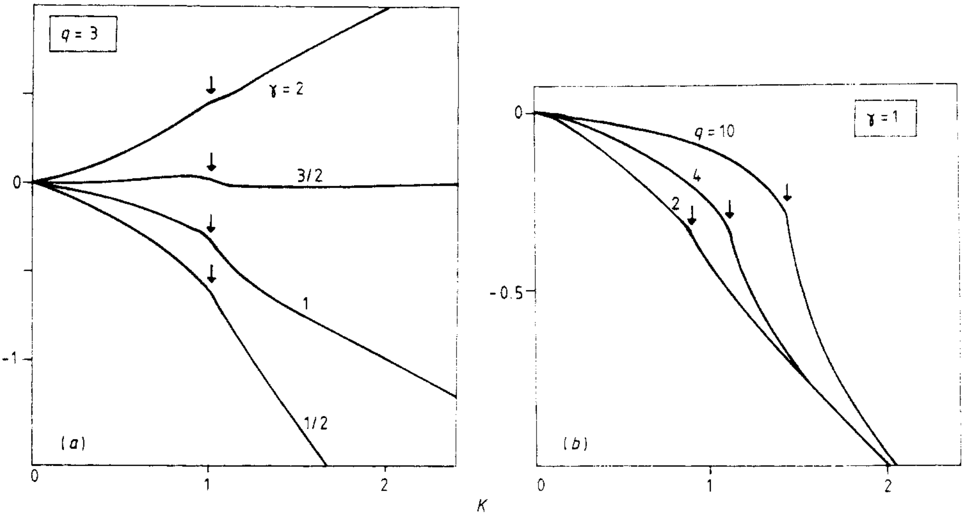

Figure 1. Surface free energies f_s for various values of q and $\gamma = K_s/K$ as obtained from the MKRG. The critical coupling constants $K^c(q)$ are indicated by small arrows.

surface free energies shown in figure 1 are neither convex nor concave. This is not an artefact of the approximation but holds also for the exact function $\bar{f}_s$.

Near to $K = K^c$, the surface free energy scales like $f_s \simeq |K - K^c|^\nu$ for $q = 2$, 3 and 4 where ν is the critical exponent of the correlation length. This implies that the surface energy $\varepsilon_s := -\mathrm{d}f_s/\mathrm{d}K$ behaves like $\varepsilon_s \simeq |K - K^c|^{\nu-1}$. For $q = 2$ (Ising case), $\nu = 1$ and the exact surface energy has a logarithmic divergence (McCoy and Wu 1973). For $q = 3$ and 4, it is now believed that $\nu = \frac{5}{6}$ and $\frac{2}{3}$ respectively (see e.g. Nienhuis *et al* 1981). Thus, for $q = 3, 4$, ε_s should diverge even stronger than in the Ising case. In the MKRG scheme, the approximate value for ν is larger than 1 in all three cases. Thus, the MKRG yields only a cusp.

Finally, we consider the effect of symmetry breaking fields on model (1). In the Ising case ($q = 2$), one bulk and one surface field are relevant at the ordinary transition. The corresponding scaling indices y_h and y_{h_1} are known exactly in $D = 2$: $y_h = \frac{15}{8}$ and $y_{h_1} = \frac{1}{2}$ (McCoy and Wu 1967). In the MKRG approach, these scaling indices are given by $y_h = 1.88$ (Migdal 1975) and by $y_{h_1} = 0.44$ (Lipowsky and Wagner 1981).

For $q \geq 3$, two symmetry breaking fields are relevant in the bulk problem. This has been discussed within the MKRG scheme by Berker and Ostlund (1979). In the semi-infinite case, we must add the following term to the Hamiltonian (1a):

$$\sum_i H_i\, \delta(\sigma_i, 1) + \sum_{\langle ij \rangle} L_{ij}\, \delta(\sigma_i, 1)\, \delta(\sigma_j, 1), \tag{8a}$$

$$H_i = \begin{cases} H_s & i \in \Lambda_s, \\ H & \text{otherwise,} \end{cases} \tag{8b}$$

$$L_{ij} = \begin{cases} L_s & i, j \in \Lambda_s, \\ L & \text{otherwise.} \end{cases} \tag{8c}$$

If we did not include the L_{ij} terms from the outset they would have been generated by the first MKRG step via the one-dimensional decimation. Within the MKRG, no other terms are generated due to the bond moving approximation.

We consider the two-dimensional case and linearise the recursion relations of the MKRG scheme around the fixed point (K^c, K_s^c). For finite rescaling factor b, these linearised recursion relations have the structure

$$\begin{pmatrix} \delta K' \\ L' \\ H' \\ \delta K_s' \\ L_s' \\ H_s' \end{pmatrix} = \begin{pmatrix} \omega_1 & 0 & \times & 0 & 0 & 0 \\ 0 & \mu_1 & \mu_2 & 0 & 0 & 0 \\ 0 & \mu_3 & \mu_4 & 0 & 0 & 0 \\ \times & 0 & \times & \omega_4 & 0 & x \\ 0 & \times & \times & 0 & \lambda_1 & \lambda_2 \\ 0 & \times & \times & 0 & \lambda_3 & \lambda_4 \end{pmatrix} \begin{pmatrix} \delta K \\ L \\ H \\ \delta K_s \\ L_s \\ H_s \end{pmatrix} \tag{9}$$

where the crosses indicate non-vanishing matrix elements which affect the eigenvectors but do not enter the eigenvalues ω_α, $\alpha = 1, 2, \ldots, 6$. ω_1 corresponds to the temperature-like perturbation $\delta K = K - K^c$ and

$$\omega_{2/3} = \tfrac{1}{2}\{\mu_1 + \mu_4 \pm [(\mu_1 - \mu_4)^2 + 4\mu_2\mu_3]^{1/2}\}$$

correspond to the symmetry breaking bulk fields H and L. ω_4 corresponds to the temperature-like perturbation $\delta K_s = K_s - K_s^c$ and

$$\omega_{5/6} = \tfrac{1}{2}\{\lambda_1 + \lambda_4 \pm [(\lambda_1 - \lambda_4)^2 + 4\lambda_2\lambda_3]^{1/2}\}$$

correspond to the symmetry breaking surface fields H_s and L_s. The scaling indices y_α are given by $y_\alpha = \ln \omega_\alpha / \ln b$. For $b = 2$, the bulk indices y_1 and $y_{2/3}$ have been calculated previously (Berker and Ostlung 1979). All bulk indices are positive. Thus, both symmetry breaking bulk fields are relevant as mentioned above. In contrast, only one surface index, namely y_5, is positive while y_4 and y_6 are negative. Thus, the MKRG scheme predicts that only one symmetry breaking surface field is relevant. For $b = 2$, we obtain the approximate values $y_5 = 0.36$ and 0.31 for $q = 3$ and 4 respectively.

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