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The Semi-Infinite Potts Model: A New Low Temperature Phase

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We consider the semi-infinite q-state Potts model in the many component limit $q \to \infty$. Both mean field theory and the Migdal-Kadanoff renormalization group scheme are used to obtain an approximate surface free energy. Both methods predict a new low temperature phase where the bulk is ordered while the free surface is disordered.

1. Introduction

The thermodynamics of the phase transition which occurs in the infinite q-state Potts model is contained in the bulk free energy f_B. The first derivative df_B/dT with respect to temperature T can be either continuous or discontinuous. For each space dimension D, there is a critical value $q^*(D)$. For $q<q^*(D)$, df_B/dT is continuous while it is discontinuous for $q>q^*(D)$. For $D=2$, $q^*(2)=4$ is known exactly [1]. For $D=3$, recent renormalization group (RG) calculations indicate $q^*(3)=3$ [e.g. [2, 3]). For a semi-infinite q-state Potts model, new types of phase transitions will occur due to the presence of a free surface. The thermodynamics of these transitions is contained in the surface free energy f_S.

For the semi-infinite Ising model ($q=2$) in dimension $D>2$, the phase diagram consists of three phases separated by three different phase boundaries [4–6]. This leads to four types of phase transitions: the ordinary, the surface, the extraordinary, and the special or surface bulk transition. The first temperature derivative df_S/dT of the surface free energy is continuous across all four types of transitions [7]. For $q>2$, no explicit calculations have appeared in the literature. Naively, we expect that the phase diagram is similar to the phase diagram of the Ising model. We also expect that the nature of the corresponding transitions should depend on q. All transitions should be continuous for $q<q^*(D)$ and discontinuous for $q>q^*(D-1)$. For $q^*(D)<q<q^*(D-1)$, the surface transition should be continuous while the other three transitions should be discontinuous.

In this paper, we are concerned with the case $q>q^*(D-1)$. We consider the extreme situation where $q \to \infty$. In this limit, approximate surface free energies can be obtained analytically both from mean field theory and from the Migdal-Kadanoff RG approach. In contrast to the naive expectation, both methods predict a new low temperature phase. In this phase, the bulk is ordered while the free surface is not. As a consequence, there exists a phase transition where the order parameter jumps in the surface while it varies smoothly in the bulk. In a forthcoming paper, we will show that this feature is not peculiar to the $q \to \infty$ limit [8].

The paper is organized as follows. First, we define the semi-infinite Potts model and its many component limit ($q \to \infty$) in Sect. 2. In Sect. 3, we extend the mean field theory which has been developed in [9] for the infinite Potts model to the semi-infinite case. In Sect. 4, we investigate the same problem by the Migdal-Kadanoff RG approach as described in [10]. Finally, we compare the results of the two methods in Sect. 5.

2. Model

Consider a D-dimensional hypercubic lattice which consists of L $(D-1)$-dimensional layers Ω_l, $l=1, 2, \ldots, L$. Potts spin variables $\sigma_i = 1, \ldots, q$ are placed on the sites i of this lattice. For each layer, periodic boundary conditions are employed for its

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$(D-1)$ Cartesian directions. The Hamiltonian of this model is given by

$$-\beta\mathscr{H}=\sum_{\langle ij\rangle}\mathscr{B}(\sigma_i,\sigma_j) \tag{2.1a}$$

$$\mathscr{B}(\sigma_i,\sigma_j)=\begin{cases}K_S\,\delta(\sigma_i,\sigma_j) & i,j\in\Omega_1,\Omega_L\\ K\,\delta(\sigma_i,\sigma_j) & \text{otherwise}\end{cases} \tag{2.1b}$$

where $\langle ij\rangle$ indicates a summation over nearest neighbours only and $\delta(\sigma_i,\sigma_j)=1$ iff $\sigma_i=\sigma_j$ and $\delta(\sigma_i,\sigma_j)=0$ otherwise.
The total free energy F is defined by

$$F(K,K_S)=\ln\sum_{\{\sigma\}}e^{-\beta\mathscr{H}}. \tag{2.2}$$

Note that the physical free energy is proportional to $-F$. Thus a lower (upper) bound for F is an upper (lower) bound for the physical quantity. The bulk free energy f_B is obtained from (2.2) via

$$f_B(K):=\lim_{N\to\infty}F(K,K_S)/N \tag{2.3}$$

where N is the total number of sites. We take the limit $L\to\infty$ in such a way that we end up with a semi-infinite system. The corresponding surface free energy f_S is given by

$$f_S(K,K_S):=\lim_{\substack{N\to\infty\\ N_S\to\infty}}(F-Nf_B)/N_S \tag{2.4}$$

where N_S is the number of sites in Ω_1 and Ω_L.
The critical temperature of the bulk transition is proportional to $\{\ln(1+\sqrt{q})\}^{-1}$ [11]. In order to obtain a sensible $q\to\infty$ limit, one has to rescale the temperature by a factor $\ln q$ [12]. Thus, we define the corresponding limit of the free energies (2.3) and (2.4) by

$$f_B^\infty(J):=\lim_{q\to\infty}f_B(J\ln q)/\ln q \tag{2.5a}$$

$$f_S^\infty(J,J_S):=\lim_{q\to\infty}f_S(J\ln q,J_S\ln q)/\ln q. \tag{2.5b}$$

The bulk free energy f_B^∞ is known exactly for all temperatures and $D\geqq 1$ [11]. The temperature derivative df_B^∞/dT has a finite jump at the bulk transition point. This behaviour is typical for all $q>q^*(D)$ [1]. By analogy, we expect that the typical features of the surface free energy f_S^∞ are valid for all $q>q^*(D-1)$.

3. Mean Field Theory

For the infinite Potts model, a mean field theory has been developed by Mittag and Stephen [9]. They introduced a real order parameter R which satisfies the selfconsistent equation

$$R=\frac{e^{2DKR}-1}{e^{2DKR}+q-1}. \tag{3.1}$$

In addition, they showed that the mean field approximation to the bulk free energy is

$$f_B(K)=\frac{DK}{q}+\frac{q-1}{q}DKR^2-Y_q(R) \tag{3.2}$$

$$Y_q(x)=-\ln q+\frac{1}{q}[1+(q-1)x]\ln[1+(q-1)x]$$
$$+\frac{q-1}{q}(1-x)\ln(1-x) \tag{3.3}$$

where R is a function of K via (3.1). In the limit $q\to\infty$ with $K=J\ln q$, (3.1) leads to $R=0$ for $J<1/2D$ and to $R=0$ or $R=1$ for $J>1/2D$. From (3.2) we obtain

$$f_B^\infty(J)=\lim_{q\to\infty}f_B(J\ln q)/\ln q=1+DJR^2-R$$
$$=\begin{cases}1 & R=0\\ DJ & R=1.\end{cases} \tag{3.4}$$

Since we have to maximize f_B^∞ with respect to R (remember that we absorbed a minus sign in the definition of f_B) we have to choose

$$R=\begin{cases}0 & J<1/D\\ 1 & J\geqq 1/D.\end{cases} \tag{3.5}$$

When (3.5) is inserted into (3.4) the exact bulk free energy in the many component limit is obtained [12]. The critical coupling constant is $J^c=1/D$. Note that $f_B^\infty(J)$ may be simply obtained from the $q\to\infty$ limit of the high and low temperature expansions.
This mean field theory can be easily generalized to the model defined by (2.1). We introduce a real order parameter R_l for each layer Ω_l. In a mean field approximation in the spirit of [9] these order parameters satisfy the following set of selfconsistent equations:

$$R_l=\frac{e^{x_l}-1}{e^{x_l}+q-1} \tag{3.6a}$$

where

$$x_l=\begin{cases}2(D-1)K_SR_1+KR_2 & l=1\\ 2(D-1)KR_l+K(R_{l-1}+R_{l+1}) & 2\leqq l\leqq L-1\\ 2(D-1)K_SR_L+KR_{L-1} & l=L\end{cases} \tag{3.6b}$$

In this case, the mean field approximation to the total free energy is

$$F=\frac{N_S}{2q}\{2(D-1)K_S+(L-2)DK+K$$
$$+(q-1)(D-1)K_S(R_1^2+R_L^2)$$
$$+(q-1)(D-1)K\sum_{1<l<L}R_l^2$$
$$+(q-1)K\sum_{1\leq l\leq L-1}R_lR_{l+1}-q\sum_{1\leq l\leq L}Y_q(R_l)\}. \tag{3.7}$$

From (3.2) and (3.7) we may obtain the surface free energy f_S via (2.4). The result is

$$f_S(K,K_S)=\{(D-1)K_S+(1/2-D)K$$
$$+(q-1)(D-1)(K_SR_1^2-KR^2)+(q-1)(D-1)K$$
$$\cdot\sum_{1<l}(R_l^2-R^2)+(q-1)K\sum_{1\leq l}(R_lR_{l+1}-R^2)$$
$$-(q-1)KR^2/2-q\sum_{1\leq l}[Y_q(R_l)-Y_q(R)]\}/q \tag{3.8}$$

where R is the order parameter of the bulk defined by (3.1). In the derivation of (3.8) we used the fact that $R_l=R_{L+1-l}$ for finite L due to reflection symmetry.

For finite q, the set of Eqs. (3.6) and (3.8) may be easily investigated on a computer [8]. Here, we are interested in the many component limit where we can solve the problem analytically. From (3.8) we obtain

$$f_S^\infty(J,J_S)=\lim_{q\to\infty}f_S(J\ln q,J_S\ln q)/\ln q$$
$$=(D-1)(J_SR_1^2-JR^2)+(D-1)J\sum_{1<l}(R_l^2-R^2)$$
$$+J\sum_{1\leq l}(R_lR_{l+1}-R^2)-JR^2/2-\sum_{1\leq l}(R_l-R). \tag{3.9}$$

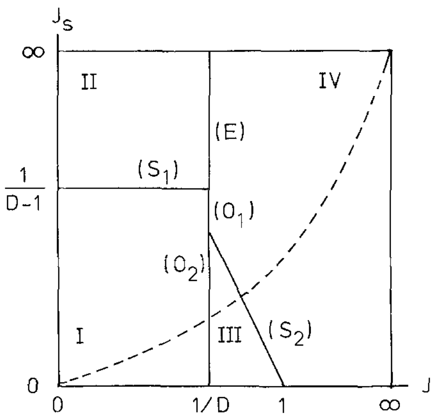

Fig. 1. Global phase diagram in mean field theory. There are four phases I, II, III, and IV separated by the phase boundaries (full curves) (S_1), (E), (O_1), (O_2), and (S_2). The broken curve indicates the physical path discussed in the text

From (3.6) we conclude that each $R_l=1$ or 0 for $q\to\infty$. For some coupling constants J and J_S, several order parameter profiles are possible. However, there is always a unique profile which maximizes the surface free energy (3.9). This leads ro four different phases denoted by I, II, III and IV in Fig. 1. The phase boundary (S_1) (see Fig. 1) which separates the phases I and II is $J_S(J)=1/(D-1)$ for $0<J<1/D$. The line $J=J^c=1/D$ separates the high temperature phases I and II from the low temperature phases III and IV. This line consists of three parts denoted by (O_1), (O_2), and (E) in Fig. 1. Finally, there is the phase boundary (S_2) between III and IV given by $J_S(J)=(1-J)/(D-1)$ with $J>J^c=1/D$. The corresponding order parameter profiles are

$$\begin{array}{lll} R_l=0; & l\geqq 1 & \text{I}\\ R_1=1,\ R_l=0; & l\geqq 2 & \text{II}\\ R_1=0,\ R_l=1; & l\geqq 2 & \text{III}\\ R_l=1; & l\geqq 1 & \text{IV}. \end{array} \tag{3.10}$$

Thus, we find a new phase (denoted by III) not present in the semi-infinite Ising model. In this phase, the bulk is ordered ($R=1$) while the surface layer is disordered ($R_1=0$).

When we insert the order parameter profiles (3.10) into (3.9) we obtain

$$f_S^\infty(J,J_S)=\begin{cases}0 & \text{I} \quad (3.11\text{a})\\ (D-1)J_S-1 & \text{II} \quad (3.11\text{b})\\ 1-(D+1/2)J & \text{III} \quad (3.11\text{c})\\ (D-1)J_S+(1/2-D)J & \text{IV}. \quad (3.11\text{d})\end{cases}$$

The expression (3.11a) valid for phase I can also be obtained from the many component limit of the high temperature expansion. Similarly, (3.11d) can be obtained from the low temperature expansion. In addition, there are two exact relations which test the validity of (3.11b) and (3.11c). If we put $J=0$, the exact surface free energy in D dimensions may be expressed by the exact bulk free energy in $(D-1)$ dimensions. In our case, this implies

$$f_S^\infty(J=0,J_S;D)=f_B^\infty(J_S;D-1)-1. \tag{3.12}$$

This exact relation is satisfied by the mean field solution (3.11) and (3.4). On the other hand, if we put $J_S=0$, the spins in the surface layer are decoupled from each other. Thus, we can do the partial trace over these spins and obtain a new semi-infinite system with surface couplings $J_S=J$. In the many component limit of model (2.1), this leads to the exact relation

$$f_S^\infty(J,J_S=0)=\begin{cases}f_S^\infty(J,J) & J<1/D\\ 1-DJ+f_S^\infty(J,J) & 1/D<J<1\\ J-DJ+f_S^\infty(J,J) & 1<J.\end{cases} \tag{3.13}$$

Again, this relation is satisfied by the mean field solution (3.11).

The unexpected feature of the mean field solution (3.11) is the appearance of the phase III. From the order parameter profiles (3.10) we know that this phase is characterized by an ordered bulk and a disordered surface. This can be deduced directly from $f_S^\infty(J, J_S)$ by looking at $e_S^\infty := \frac{\partial}{\partial J_S} f_S^\infty(J, J_S)/(D-1)$. This quantity is the correlation function of two surface spins which are nearest neighbours. From (3.13) we obtain

$$e_S^\infty = \begin{cases} 0 & \text{I, III} \\ 1 & \text{II, IV.} \end{cases} \tag{3.14}$$

Thus, for phase III there are no correlations in the surface layer.

Due to this phase, a new type of phase transition occurs in the low temperature regime. Consider the physical trajectory indicated by the broken curve in Fig. 1. This curve represents the path $J_S(J) = J/2$ where J is proportional to the inverse temperature. Let's start at high temperatures in phase I. When we lower the temperature we first cross the phase boundary (O_2) (see Fig. 1). At this temperature, the bulk order sets in and all layers are ordered except for the surface layer. If we lower the temperature even more a second phase transition occurs as soon as we cross the phase boundary denoted by (S_2) in Fig. 1. At the corresponding "critical" temperature the order parameter R_1 of the surface layer jumps from $R_1 = 0$ to $R_1 = 1$. At this point, one may wonder if this behaviour is just peculiar to the many component limit ($q \to \infty$). However, the mean field equations (3.6) and (3.8) predict a similar behaviour for finite q [8].

The surface free energy (3.11) along the physical trajectory just discussed is depicted in Fig. 2. Thus, we observe that the surface free energy has a jump at the phase transition (O_2) while it is continuous at (S_2). The jump at (O_2) is not peculiar to the physical trajectory chosen above. It is easily verified that f_S^∞ has a jump along the whole line $J = J^c = 1/D$ except for the point $(J, J_S) = (J^c, J_S^c)$ with $J_S^c = (1 - 1/2D)/(D-1)$. We don't know whether this feature is an artefact of the mean field approximation. There seems to be no general theorem which excludes such a behaviour. The surface energy $\varepsilon_S^\infty := \frac{d}{dJ} f_S(J, J_S(J))$ along the physical path $J_S(J) = J/2$ is shown in Fig. 2b. Both at the transition (O_2) and at (S_2), this quantity has a finite jump as a function of temperature.

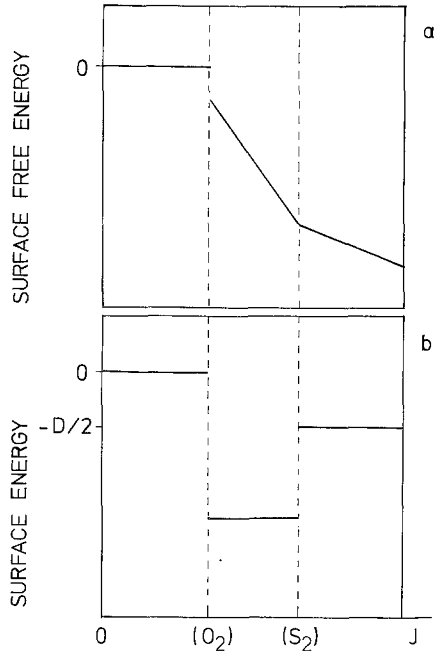

Fig. 2a and b. Mean field result for **a** surface free energy and **b** surface energy along the physical path indicated in Fig. 1

4. Migdal-Kadanoff RG

Various position space renormalization group methods have been used to discuss the semi-infinite Ising model ($q=2$) [e.g. 6, 7]. Recently, it has been shown that the simple Migdal-Kadanoff renormalization group (MKRG) scheme is also adequate [10]. We now apply this scheme to the semi-infinite Potts model. For finite q, the MKRG scheme yields recursion relations both for the coupling constants K, K_S and for the bulk and surface free energies f_B, f_S which depend on q explicitely. Thus, we can take the limit $q \to \infty$ directly in these recursion relations. As a result, we obtain recursion relations for the rescaled coupling constants J, J_S and for the free energies f_B^∞, f_S^∞ defined in (2.5).

First, we discuss the bulk free energy f_B^∞ within the MKRG scheme. At each RG step, we move bonds in all D Cartesian directions simultaneously. Thus, we avoid the generation of anisotropic coupling constants (for a review on the MKRG scheme in general, see [13]). For finite rescaling factor b, we arrive at

$$J' = \begin{cases} 0 & 0 \leqq J < b^{-(D-1)} - b^{-D} \\ b^D J - b + 1 & b^{-(D-1)} - b^{-D} \leqq J < b^{-(D-1)} \\ b^{(D-1)} J & b^{-(D-1)} \leqq J \end{cases} \tag{4.1}$$

for the bulk coupling constant in the limit $q \to \infty$. For $D=2$ and $b=2$, this recursion relation has been derived previously in [14]. In the infinitesimal rescaling limit $b \to 1+\delta l$, (4.1) implies the differential recursion relation

$$\frac{dJ}{dl}=\begin{cases}0 & J=0\\ DJ-1 & 0<J<1\\ (D-1)J & 1\leqq J.\end{cases} \quad (4.2)$$

For finite b, there is one non trivial fixed point at $J^c=(b-1)/(b^D-1)$. For $b\to 1+\delta l$, $J^c=1/D$ which is exact for all $D>1$ [12]. For $D=1$, the RG flow is peculiar since there is a line of fixed points for $1<J<\infty$. However, the integration of the bulk free energy along trajectories in $D=1$ (see (4.6) below) leads to the exact result that there is only one phase transition point at $J=1$. The thermal scaling index is $y_t=D$ for all b which is exact since the bulk transition is discontinuous [15].

The corresponding recursion relation for the bulk free energy f_B^∞ is

$$f_B^\infty(J')=b^D f_B^\infty(J)-D\bar{\Delta}_B(b^{D-1}J)$$
$$-b^D+D(b-1)+1 \quad (4.3\text{a})$$

$$\bar{\Delta}_B(x)=\begin{cases}b-1 & 0\leqq x<1\\ x(b-1) & 1\leqq x\end{cases} \quad (4.3\text{b})$$

for finite b and

$$\frac{df_B^\infty}{dl}=D\{f_B^\infty-D\Delta_B(J)\} \quad (4.4\text{a})$$

$$\Delta_B(J)=\begin{cases}1 & 0\leqq J<1\\ J & 1\leqq J\end{cases} \quad (4.4\text{b})$$

for $b\to 1+\delta l$. In order to specify a solution to (4.4) we choose the boundary condition

$$\lim_{l\to\infty} l^{-Dl} f_B^\infty\{\tilde{J}(l,J)\}=0. \quad (4.5)$$

$\tilde{J}(l,J)$ is the solution of the recursion relation (4.2) with the initial condition $\tilde{J}(0,J)=J$. Integration of (4.4) with the boundary condition (4.5) yields

$$f_B^\infty(J)=D\int_0^\infty dl\, e^{-Dl}\Delta_B\{\tilde{J}(l,J)\}$$
$$=\begin{cases}1 & 0\leqq J<1/D\\ DJ & 1/D\leqq J\end{cases} \quad (4.6)$$

which is the exact bulk free energy [12]. For finite b, one obtains from (4.3)

$$f_B^\infty(J)=\begin{cases}1 & 0\leqq J<J^c=(b-1)/(b^D-1)\\ 1+D(J-J^c) & J^c\leqq J\end{cases}$$

which is an upper bound to the exact solution (4.6).

Next, we use the MKRG scheme to calculate an approximate surface free energy f_S^∞. This is done in the same way as described in [10] for the semi-infinite Ising model. The calculation of f_B^∞ indicates that it is advantageous to use the infinitesimal rescaling limit $b\to 1+\delta l$. In this limit, the recursion relation for the surface coupling J_S becomes

$$\frac{dJ_S}{dl}=\begin{cases}0 & J<2,\ J_S=0\\ (D-1)J_S+\frac{1}{2}J-1 & 0<J_S<1\\ (D-2)J_S+\frac{1}{2}J & 1\leqq J_S.\end{cases} \quad (4.7)$$

For $D>2$, the recursion relations (4.7) and (4.2) lead to three nontrivial fixed points at $(J,J_S)=(0,1/(D-1))$, $(1/D,0)$, and $(1/D,J_S^c)$ with $J_S^c=(1-1/(2D))/(D-1)$. In addition, there are three trivial ones: the high temperature fixed point at $(0,0)$, the bulk ferromagnetic one at (∞,∞), and the surface ferromagnetic one at $(0,\infty)$. $D=2$ is special since there is an additional line of fixed points for $J=0$ and $J_S>1$. This feature of the MKRG transformation is exact since for $J=0$ we have a 1-dimensional bulk system with coupling constant J_S (compare (4.2) with D replaced by $(D-1)$). However, the line of fixed points is not related to any phase transition since it is reached by integrating along trajectories up to a finite value of l.

The differential recursion relation for the surface free energy f_S^∞ is

$$\frac{df_S^\infty}{dl}=(D-1)f_S^\infty+\Delta_S(J,J_S). \quad (4.8\text{a})$$

In the inhomogeneous term Δ_S, the bulk free energy f_B^∞ enters (compare [10]). For $0<J_S<1$, this term is given by

$$\Delta_S(J,J_S)=\begin{cases}0 & 0\leqq J<1/D\\ (1-DJ)/2 & 1/D\leqq J<1\\ (D-1)(J/2-1) & 1\leqq J.\end{cases} \quad (4.8\text{b})$$

For $J_S>1$, we obtain

$$\Delta_S(J,J_S)$$
$$=\begin{cases}(D-1)(1-J_S) & 0\leqq J<1/D\\ -(D-1)J_S-DJ/2+D-1/2 & 1/D\leqq J<1\\ (D-1)J/2-(D-1)J_S & 1\leqq J.\end{cases} \quad (4.8\text{c})$$

Integration of the recursion relation (4.8a) yields

$$f_S^\infty(J,J_S)=C_S(J,J_S)-\int_0^\infty dl\, e^{-(D-1)l}\Delta_S(l) \quad (4.9\text{a})$$

$$C_S(J,J_S)=\lim_{l\to\infty} e^{-(D-1)l} f_S^\infty\{\tilde{J}(l,J),\tilde{J}_S(l,J,J_S)\}. \quad (4.9\text{b})$$

In order to specify the solution (4.9a) we have to choose boundary conditions (4.9b) for the various fixed points reached in the limit $l \to \infty$. We take

$$C_S(J, J_S) = \begin{cases} 0 & J=0, \; J_S=0 \qquad (4.10\text{a}) \\ 0 & J=0, \; J_S=\infty \qquad (4.10\text{b}) \\ -\frac{1}{2}DJ & J=\infty, \; J_S=\infty. \qquad (4.10\text{c}) \end{cases}$$

At the bulk ferromagnetic fixed point ($J, J_S \to \infty$), the boundary condition (4.10c) is necessary in order to make the scheme self-consistent [10]. With the above choice of boundary conditions, the surface free energy (4.9a) is obtained after some tedious but straightforward integrations along trajectories. As a result, five distinct phases denoted by I, II, III_1, III_2, IV in Fig. 3 are obtained. As in mean field theory, the line $J=J^c=1/D$ separates the high temperature phases (I, II) from the low temperature phases (III_1, III_2, IV). This line consists of two parts denoted by (E) and (O) in Fig. 3. The other phase boundaries indicated in Fig. 3 are

$$J_S(J) = \begin{cases} \frac{1}{2}J + \{D^\phi (J^c - J)^\phi + 1\}/\{2(D-1)\} & (\mathrm{S}_1) \\ (J-J^c)/2 + J_S^c + A(J-J^c)^\phi/(D-1) & (\mathrm{S}_2) \\ 1/(D-1) + J\{\ln(J/2) - 1\}/\{2(D-1)\} & (\mathrm{S}_2') \end{cases} \qquad (4.11)$$

with $J^c = 1/D$, $J_S^c = (1-1/(2D))/(D-1)$, $A := D^\phi (D-1)^{-\phi}(1-\ln 2 - D)/2$, and $\phi := (D-1)/D$. For $0 < J < J^c$, the surface free energy f_S^∞ as obtained from (4.9a) is

$$f_S^\infty(J, J_S) = \begin{cases} 0 & \mathrm{I} \qquad (4.12\text{a}) \\ (D-1)(J_S - J/2) - D(J^c-J)^\phi/2 - 1/2 & \mathrm{II} \qquad (4.12\text{b}) \end{cases}$$

and for $J > J^c$, it is

$$f_S^\infty(J, J_S) = \begin{cases} A(J-J^c)^\phi - D(J-J^c)/2 & \mathrm{III}_1 \qquad (4.12\text{c}) \\ -DJ + J\ln(J/2)/2 + 1 & \mathrm{III}_2 \qquad (4.12\text{d}) \\ (D-1)J_S + (1/2 - D)J & \mathrm{IV}. \qquad (4.12\text{e}) \end{cases}$$

As in mean field theory, (4.12a) and (4.12e) are the many component limits of the high and the low temperature expansions respectively. The exact relation (3.12) is satisfied by (4.12b) while the exact relation (3.13) is only satisfied for $J < 1/D$ and $J > 2$. This implies that (4.12c) and (4.12d) can't be exact.

The correlation function of two nearest neighbour surfaces spins as obtained from (4.12) is

$$e_S^\infty(J, J_S) = \begin{cases} 0 & \mathrm{I}, \mathrm{III}_1, \mathrm{III}_2 \\ 1 & \mathrm{II}, \mathrm{IV}. \end{cases} \qquad (4.13)$$

Thus, the MKRG scheme predicts that the surface layer is disordered for the low temperature phases III_1 and III_2. It is remarkable that these phases arise within a RG calculation. Although there is no fixed point at $(J, J_S) = (2, 0)$ the phase boundaries denoted by (S_2) and (S_2') in Fig. 3 connect (J^c, J_S^c) and (2, 0).

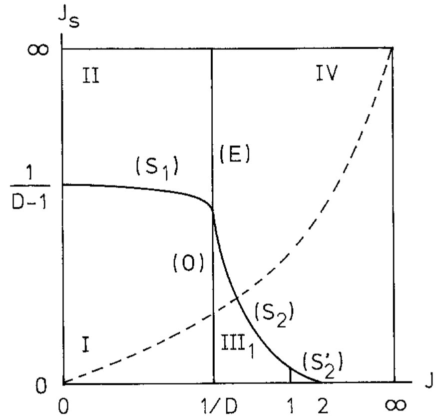

Fig. 3. Global phase diagram from the MKRG scheme. There are five phases I, II, III_1, III_2, and IV. The phase III_2 corresponds to the small triangle above $J=1$ and $J=2$. The full curves represent phase boundaries while the broken curve represents the physical path discussed in the text

The reason is that the recursion relation (4.7) is not analytic at $J_S=0$. As a consequence, the trajectories are not smooth but have a kink at $J_S=0$ and $J^c < J < 2$. In a different context, such a situation has been discussed in [16].

The surface free energy (4.12) as obtained within the MKRG scheme is continuous for all values of the coupling constants J, J_S. However, due to the terms proportional to $|J-J^c|^\phi$ in (4.12) with $\phi=(D-1)/D$ the surface energy ε_S^∞ has a rather peculiar behaviour. For instance, consider the physical path $J_S(J) = J/2$ as indicated in Fig. 3 by a broken line. The same path has been considered in Sect. 3 (compare Fig. 1). The surface free energy f_S^∞ and the

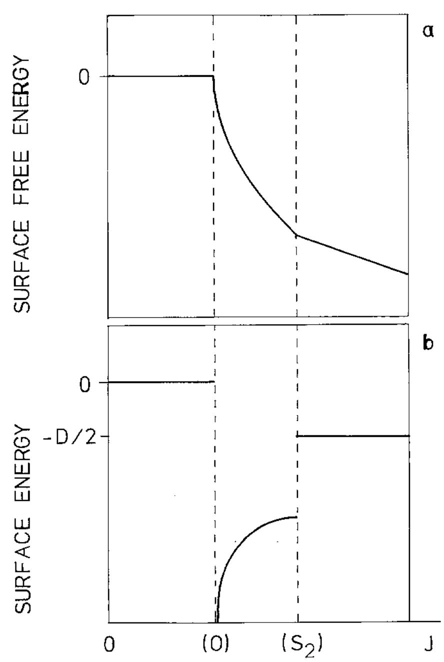

Fig. 4a and b. MKRG result for **a** surface free energy and **b** surface energy along the physical path indicated in Fig. 3

surface energy ε_S^∞ along this path are shown in Fig. 4a and b respectively. As in mean field theory, there are two phase transitions ((O) and (S_2) in Fig. 4). In contrast to the mean field result (compare Fig. 2a) f_S^∞ is a continuous function of J. At (S_2), ε_S has a jump just as in mean field theory (compare Fig. 2b). However, at (O) this quantity diverges like $(J-J^c)^{\phi-1}=(J-J^c)^{-1/D}$. Such a singularity is not ruled out on general grounds. For instance, if the transition were continuous ε_S would behave like $|J-J^c|^{D\nu-1}$ where ν denotes the critical exponent of the correlation length. In the 2-dimensional Ising model ($q=2$) where $\nu=1$ the exact ε_S has a logarithmic divergence [17]. For $q=3,4$ and $D=2$, one expects $\nu=5/6$, $2/3$ [3, 18]. Thus, ε_S should diverge even stronger in these cases. However, in our case ($q\to\infty$) the bulk transition is discontinuous. Therefore, the behaviour shown in Fig. 4b is rather unusual and may be an artefact of the bond moving approximation.

5. Summary

From the above calculations, we conclude that there exists a new low temperature phase in the many component limit of the semi-infinite Potts model (denoted by III in Fig. 1 and Fig. 3). However, both for this phase and for the high temperature phase II, the mean field and the MKRG predictions for the surface free energy f_S^∞ disagree. As far as the exact relations (3.12) and (3.13) are concerned, the mean field result (3.11) could be exact. However, (3.11) implies that f_S^∞ has a finite jump at $J=J^c$. On the other hand, the MKRG scheme leads to a surface free energy (4.12) which is continuous. But (4.12) can't be exact since it does not satisfy the rigorous relation (3.13) for all J.

Mean field theory yields a lower bound to the total free energy F (remember the sign convention in (2.2)). In addition, the mean field result for the bulk free energy f_B^∞ is exact. Thus, we expect that (3.11) is a lower bound to the exact f_S^∞. On the other hand, the differential MKRG scheme also yields the exact bulk free energy f_B^∞. In addition, for the semi-infinite Ising model ($q=2$) the MKRG approximation gives an upper bound to the total free energy F [10]. Thus, we might hope that the MKRG result (4.12) is an upper bound to the exact f_S^∞. For $D=2$, this expectation is consistent with (3.11) and (4.12) since

$$f_S^\infty[\text{Mean Field}] \leqq f_S^\infty[\text{MKRG}], \quad D=2 \tag{5.1}$$

for all coupling constants J, J_S. However, for $D>2.17$ this inequality does not hold for phase III.

Finally, we mention a simple mean field type of argument which leads to the new phase III without any calculation. Consider the surface layer Ω_1 with coupling constant J_S. We approximate the effect of the second layer Ω_2 on Ω_1 by an effective field h_{eff} which is

$$h_{\text{eff}} \simeq \begin{cases} 0 & J<1/D \\ J & J \geqq 1/D. \end{cases} \tag{5.2}$$

Thus, we have a $(D-1)$-dimensional bulk model in the presence of an external field. For $q\to\infty$, the bulk free energy f^∞ of this problem is known exactly [12]:

$$f^\infty = \begin{cases} 1 & (D-1)J_S+h_{\text{eff}}<1 \\ (D-1)J_S+h_{\text{eff}} & (D-1)J_S+h_{\text{eff}}>1. \end{cases} \tag{5.3}$$

(5.3) shows that the surface is disordered even in the presence of an effective magnetic field h_{eff} as long as $J_S<(1-h_{\text{eff}})/(D-1)$. If we express h_{eff} by J via (5.2) we find that the surface is disordered for $J>1/D$ and $J_S<\frac{1-J}{D-1}$. This is just the phase III found in the meanfield calculation of the semi-infinite problem (see Fig. 1).

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