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LETTER TO THE EDITOR

Interface method for the antiferromagnetic three-state Potts model on a square lattice†

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Abstract. A generalised version of the interface method of Müller-Hartmann and Zittartz is applied to the three-state square lattice Potts antiferromagnet in a negative field. The phase boundary is found to go to zero temperature in the limit of zero magnetic field.

The interface method developed by Müller-Hartmann and Zittartz (1977) has turned out to be a very precise approximation for calculating the phase boundary of Ising models with ferromagnetic, antiferromagnetic and even competing interactions on the square lattice (Müller-Hartmann and Zittartz 1977, Burkhardt 1978, Hornreich *et al* 1979, Kroemer and Pesch 1982). The method has been extended and applied to the triangular Ising antiferromagnet (Lin and Wu 1979, Dóczy-Réger and Hemmer 1981) and the limits of its applicability have also been investigated by Lin and Wu (1979) who found that only a generalised version could be applied to systems like the Potts, eight-vertex and Ashkin-Teller models.

In this letter we study the antiferromagnetic three-state Potts model on a square lattice in the presence of a magnetic field defined by the Hamiltonian

$$H = J \sum_{(i,j)} \delta_{S_i S_j} - h \sum_i \delta_{S_i 0}$$

where the first sum runs over all nearest-neighbour pairs and the second over all the lattice sites. $S_i = -1, 0, +1$ is one of the three states and $\delta_{S_i S_j}$ is the Kronecker delta function. The interaction energy J is positive and we restrict ourselves to a negative field $h < 0$. In this case the $S_i = 0$ state is energetically unfavourable and the system has the double degenerate ground state of an Ising antiferromagnet.

Because of the simple ground state properties, the method of Müller-Hartmann and Zittartz can be easily applied. The interface free energy σ is defined by

$$\sigma = -(kT/N) \ln(Z_I/Z_H) \quad (1)$$

where a periodic boundary condition is taken in the horizontal direction and Z_I (Z_H) is the partition function with different (the same) boundary conditions at the bottom

† A preliminary version of this work has been presented at the Ninth International Seminar on Phase Transitions and Critical Phenomena, April 13-5, 1982, Vienna, Austria.

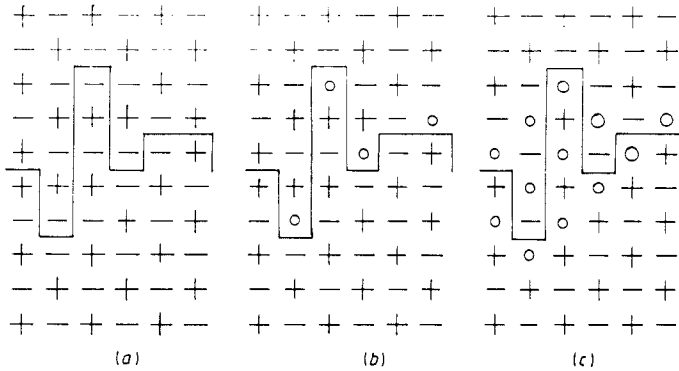


Figure 1. Typical interface configurations for the three-state antiferromagnetic Potts model in a negative field. (a) $h = -\infty$; (b) h is finite; (c) $-h \ll J$.

and on the top of the system (see figure 1). The lattice consists of N columns. The critical condition is determined by $\sigma = 0$ since the interface free energy becomes zero at a continuous phase transition. Like Müller-Hartmann and Zittartz (1977), we approximate Z_I by considering only a special class of configurations with a single interface crossing each column just once. Typical cases are shown in figure 1 for three different values of the field. When $h = -\infty$ the Potts model becomes just the Ising antiferromagnet without any magnetic field, and in this case the interface method gives the exact σ and T_c (Müller-Hartmann and Zittartz 1977). In a finite field, spins in the state 0 will appear at the interface to destroy some of the ferromagnetic bonds. In the limit $-h \ll J$ all the ferromagnetic bonds along the interface are removed by turning a spin on one chosen sublattice into the state 0 (see figure 1 (c)). We note that without taking into account configurations just described we would get a phase boundary independent of the field, obviously an incorrect result.

The interface method has been applied recently by Selke and Pesch (1982) to the case of the ferromagnetic three-state Potts model without magnetic field. This system has a triple degenerate ground state and its interface properties are quite different from those in the antiferromagnetic case. In Selke and Pesch's approach, spins in the third state appear in domains between the two ordered phases, thus giving rise to a gain in entropy but not in energy.

Before going into the details of the calculation, let us consider some problems concerning the phase boundary of our model. The partition function of the three-state antiferromagnetic Potts model is known exactly in a limiting case. If the temperature and magnetic field approach zero while their ratio $R = kT/h$ remains finite, the partition function becomes

$$Z = \sum' (e^{R^{-1}})^{N_0} \quad (2)$$

where the prime means that configurations are restricted to those without nearest-neighbour spins in the same state and N_0 is the number of spins in the state 0. Equation (2) is a special case of the three-colouring problem that was solved exactly by Baxter (1970) who found a continuous transition at the activity $e^{R^{-1}} = 1$. That means the phase boundary must go to zero temperature with an infinite slope as h approaches zero. Of course, this does not exclude the possibility of one or more transition temperatures in zero field as proposed by Grest and Banavar (1981) and Cardy (1981),

following a suggestion by Berker and Kadanoff (1980) that a system with sufficiently complex macroscopically degenerate ground state, like the three-state Potts model on d -dimensional hypercubic lattices, may have a finite-temperature transition from a paramagnetic to a massless phase. Using the phenomenological renormalisation-group method Nightingale and Schick (1982), however, came to the conclusion that zero is the only transition temperature. This was confirmed by a Monte Carlo renormalisation-group calculation made by Jayaprakash and Tobochnik (1982). That suggests a phase diagram like that displayed in figure 2(a). The interface method of

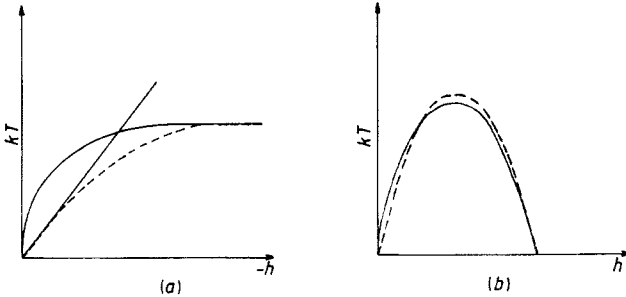


Figure 2. (a) Expected phase boundary for the three-state antiferromagnetic Potts model on a square lattice in a negative field (full line). The broken line could be obtained by the interface method in finite field. Its slope at $T = 0$ was calculated in the text. (b) Phase boundary of the triangular Ising antiferromagnet. The infinite slope of the full line at $T = 0$ was argued to be exact by Kinzel and Schick (1981), while the broken line was obtained by the interface method (Dóczy-Réger and Hemmer 1981).

the present letter supports the result of Nightingale and Schick (1982) and Jayaprakash and Tobochnik (1982), providing a phase boundary that goes to zero temperature, as $h \rightarrow 0^-$, with the slope

$$R = kT/h = -1.113. \tag{3}$$

The finiteness of R seems to be the consequence of the approximation of taking into account only special interface configurations in computing Z_I . The situation is quite similar to the case of the triangular Ising antiferromagnet. Both models have a macroscopically degenerate ground state in zero magnetic field. T_c is exactly known to be zero in the Ising system (Houtappel 1950) and, according to scaling arguments (Kinzel and Schick 1981), the slope of the phase boundary is infinite (see figure 2(b)). The interface method, however, gives a finite slope (Dóczy-Réger and Hemmer 1981).

Finally, we proceed to compute our result for R (equation (3)) using the transfer matrix method. Because of the calculational difficulties, we confine ourselves to the limit $-h \ll J$. In that case

$$Z_I = 2 \sum_{\{n_i\}} \exp\left(\frac{h}{kT} \sum_{i=1}^N k_i\right) \tag{4}$$

where k_i is the number of spins in the state 0 belonging to the i th column and the factor 2 arises because of the two sublattices. In order to define the transfer matrix, we describe a configuration by the numbers $\{n_i\} = \{n_1, n_2, \dots, n_N\}$, where n_i defines the place of the interface in the i th column with respect to the reference interface (figure 3). There is a danger of overcounting, since for a given configuration the

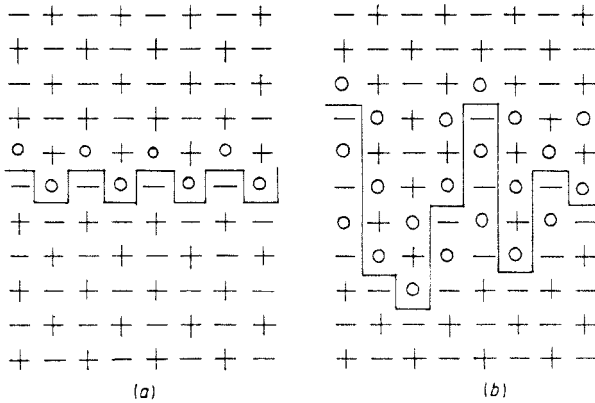


Figure 3. (a) The reference interface $\{n_i\} = \{1, 0, 1, 0, 1, 0, 1, 0\}$. (b) The configuration $\{n_i\} = \{3, -2, -3, 0, 3, -2, 1, 0\}$.

interface lines can be drawn in 2^N ways. If n_i is defined to be even (odd) for i even (odd), then the overcounting is avoided (see example on figure 3(b)). It should be stressed that J is missing from (4) since all the ferromagnetically ordered bonds have been removed. k_i depends not only on n_i but on n_{i-1} and n_{i+1} as well, so we have actually a three-body interaction problem. We refer to figure 4 where $k_i(n_{i-1}, n_i, n_{i+1})$ is given explicitly for the two basic situations. The transfer matrix \mathbf{T} can be defined by

$$T_{n_1, n_2; n_3, n_4} = \exp[h(k_2 + k_3)/kT],$$

and then

$$Z_I = 2 \text{Tr}\{\mathbf{T}^{N/2}\}.$$

Using equation (1),

$$\sigma = -\frac{1}{2}kT \ln \lambda$$

where λ is the largest eigenvalue of \mathbf{T} . Here the obvious fact that $Z_H = 1$ has been used.

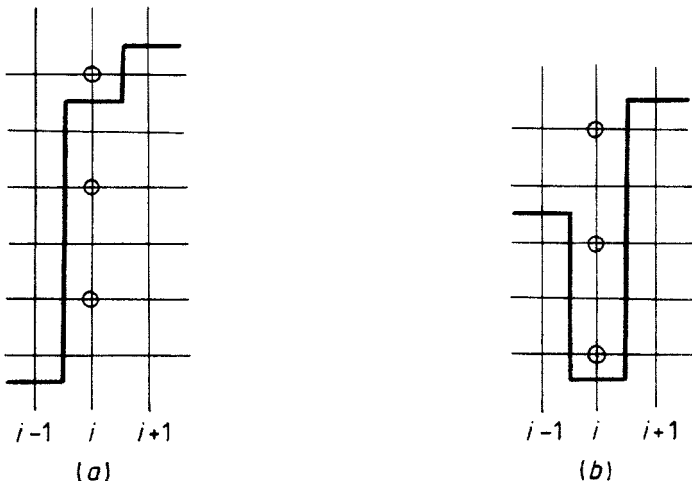


Figure 4. The number of spins k_i in the state 0 for the two basic cases. (a) $2k_i = |n_{i+1} - n_{i-1}|$; (b) $2k_i = \max\{|n_{i+1} - n_i|; |n_i - n_{i-1}|\} + 1$.

Our aim is to find an eigenvector of \mathbf{T} consisting only of positive elements. Then it follows from the Perron–Frobenius theorem that the corresponding eigenvalue must be the largest one. Inspecting the form and the symmetries of \mathbf{T} suggests the following sum as an eigenvector:

$$f = \sum_{i=1}^{\infty} a_i f_i \quad (5)$$

with

$$(f_i)_{n_1, n_2} = \exp[(lh/2kT)|n_1 - n_2|], \quad l = 1, 2, 3, \dots$$

The effect of \mathbf{T} on f_l can be obtained by a straightforward but somewhat tedious calculation

$$\mathbf{T}f_l = c_{1,l}f_1 + c_{2,l}f_2 + c_{l+2,l}f_{l+2} \quad (6)$$

where the coefficients c as functions of h/kT were explicitly computed. Putting (5) into the eigenvalue equation $\mathbf{T}f = \lambda f$ and using (6), the following equations for λ and the a_i are derived:

$$\lambda a_1 = \sum_{i=1}^{\infty} c_{1,i} a_i, \quad \lambda a_2 = \sum_{i=1}^{\infty} c_{2,i} a_i, \quad \lambda a_l = c_{l,l-2} a_{l-2}, \quad l = 3, 4, 5, \dots$$

Making use of the simple recursion relation of the last row, only two of the equations remain:

$$\begin{aligned} \lambda a_1 &= \left(c_{1,1} + \sum_{i=1}^{\infty} c_{1,2l+1} A_i \lambda^{-i} \right) a_1 + \left(c_{1,2} + \sum_{i=1}^{\infty} c_{1,2l+2} B_i \lambda^{-i} \right) a_2, \\ \lambda a_2 &= \left(c_{2,1} + \sum_{i=1}^{\infty} c_{2,2l+1} A_i \lambda^{-i} \right) a_1 + \left(c_{2,2} + \sum_{i=1}^{\infty} c_{2,2l+2} B_i \lambda^{-i} \right) a_2, \end{aligned} \quad (7)$$

where

$$A_l = \prod_{j=1}^l c_{2j+1,2j-1}, \quad B_l = \prod_{j=1}^l c_{2j+2,2j}, \quad l = 1, 2, 3, \dots$$

From (7) (which was solved by using a computer for several values of h/kT) we get an eigenvector f with positive elements only. Thus the corresponding eigenvalue λ can be used to calculate the interface free energy σ , and the critical condition (3) comes from setting $\sigma = 0$ ($\lambda = 1$).

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