About the critical condition of the spin S=1 Ising model on the anisotropic square and SC lattice

1987 J. Phys. A: Math. Gen. 20 6147

(http://iopscience.iop.org/0305-4470/20/17/049)

J. Phys. A: Math. Gen. 20 (1987) 6147-6149. Printed in the UK

COMMENT

About the critical condition of the spin $S=1$ Ising model on the anisotropic square and SC lattice

I M Savić† and Lj Maurer‡

† Department of Physics and Meteorology, Faculty of Natural and Mathematical Sciences, University of Belgrade, PO Box 550, 11001 Belgrade, Yugoslavia
‡ Institute of Mathematics and Physics, 81000 Titograd, Yugoslavia

Received 25 March 1987, in final form 2 June 1987

Abstract. We extend to the $S=1$ Ising model a simple procedure which was proposed recently for the q-state Potts model. The approximate critical conditions are obtained for the ferromagnetic model on the square and simple cubic lattice.

The model considered in this comment is the spin $S=1$ Ising ferromagnet with different two-site interactions along different lattice axes. For such an Ising model on a lattice of N sites, the Hamiltonian $\mathscr{H}$ generally takes the form

$$\mathscr{H} = -\sum_{\alpha=1}^{p} J_\alpha \sum_{\langle ij\rangle} S_i S_j. \tag{1}$$

Here $S_i=-1,0,1$ specifies the spin state at the ith site, $J_\alpha > 0$ is the strength of the two-site interaction along the α axis ($\alpha = 1, 2, 3, \ldots, p$) and the sum is taken over the nearest-neighbour sites on the lattice. To our best knowledge there are no exact critical conditions available for anisotropic models in $d \geqslant 2$ dimensions.

In this comment we are going to extend to the spin $S=1$ model a simple method (Hajduković 1983, Hajduković and Šćepanović 1986) which is known to be very accurate for the spin $S=\frac{1}{2}$.

To this end let us rewrite the Hamiltonian (1) in the form

$$\mathscr{H} = -\sum_{\alpha=1}^{p} J_\alpha n_\alpha + \sum_{\alpha=1}^{p} J_\alpha m_\alpha \tag{2}$$

where n_α is the number of bonds along the α axis ($\alpha = 1, 2, \ldots, p$) with both ends in the $S_i=1$ or both ends in $S_i=-1$ state. Similarly m_α is the number of bonds with one end in the $S_i=+1$ state and the other in the $S_i=-1$ state. The partition function is then

$$Z = \sum_{\{n,m\}} G(n_1, n_2, \ldots, n_p, m_1, m_2, \ldots, m_p) \exp\left(\sum_{\alpha=1}^{p} K_\alpha (n_\alpha - m_\alpha)\right)$$
$$\equiv \sum_{\{n,m\}} z(n_1, n_2, \ldots, n_p, m_1, m_2, \ldots, m_p). \tag{3}$$

Here $K_\alpha \equiv J_\alpha / k_B T$, the sum is taken over all possible values of $n_1, n_2, \ldots, n_p$, $m_1, m_2, \ldots, m_p$ and $G(n_1, \ldots, n_p, m_1, \ldots, m_p)$ is the number of configurations for a given sequence $\{n_1, \ldots, n_p, m_1, \ldots, m_p\}$.

To be definite let us consider the case of a square lattice with couplings K_1 and K_2 along two different lattice axes. It is extremely difficult to obtain $z(n_1, n_2, m_1, m_2)$ for the entire lattice. They are, however, easily obtained for just a single square. As shown in the previous paper (Hajduković and Šćepanović 1986) in the case $S=\frac{1}{2}$, information about the critical condition of the infinite system is retained in the values of $z(n_1, n_2, m_1, m_2)$ for a single square. In fact, for the spin $S=\frac{1}{2}$ model we have equalities

$$n_1+m_1=2 \qquad n_2+m_2=2. \tag{4}$$

The possible values of $z(n_1, n_2, m_1, m_2)$ are $z(2, 2, 0, 0)$, $z(1, 1, 1, 1)$, $z(2, 0, 0, 2)$, $z(0, 2, 2, 0)$, $z(0, 0, 2, 2)$ and the exact critical condition for the $S=\frac{1}{2}$ square lattice is

$$z(2,2,0,0)-z(1,1,1,1)-z(2,0,0,2)-z(0,2,2,0)+z(0,0,2,2)=0. \tag{5}$$

So, for $S=\frac{1}{2}$ the exact critical condition (5) is a linear combination of all functions $z(n_1, n_2, m_1, m_2)$ permitted by equations (4). In the case $S=1$, instead of equalities (4), we have inequalities

$$\begin{aligned} 0 \leqslant n_1+m_1 \leqslant 2 \\ 0 \leqslant n_2+m_2 \leqslant 2 \end{aligned} \tag{6}$$

because of the fact that some of the bonds may have one or both ends in the state $S_i=0$. Thus we have new possible values for $z(n_1, n_2, m_1, m_2)$ and we shall suppose that the exact critical condition for the $S=1$ model differs from (5) only in the right-hand side, which is now not zero but some linear combination L of these new possible values $z(n_1, n_2, m_1, m_2)$. However, we do not know an actual rule to form the linear combination needed with these new values of $z(n_1, n_2, m_1, m_2)$.

So we shall give some intuitive arguments in order to obtain an approximation for the needed linear combination L. The characteristic of states permitted by (4) is that both ends of every bond are in a state $S_i \neq 0$. These states correspond to the right-hand side of intervals (6). On the other hand bonds of this type are not possible on a single square (or in general on a hypercube in d dimensions) only if the number of spins in the zero spin state is greater or equal to 2^d-1, where 2^d is the number of sites of a hypercube in d dimensions. The corresponding sum of values $z(n_1, n_2, m_1, m_2)$ for 2^d and 2^d-1 spins in the zero state is

$$L=1+2^{d+1}. \tag{7}$$

We shall use (7) as an approximation for a needed linear combination. In other words, we ignore the values $z(n_1, n_2, m_1, m_2)$ inside intervals (6). As a consequence our approximate critical condition for the $S=1$ model is of the same form as (5) with constant right-hand side determined by (7). In explicit form for $S=1$ we have

$$\begin{aligned} z(2,2,0,0) &= 2\exp(2K_1+2K_2) \\ z(1,1,1,1) &= 8 \\ z(2,0,0,2) &= 2\exp(2K_1-2K_2) \\ z(0,2,2,0) &= 2\exp(2K_2-2K_1) \\ z(0,0,2,2) &= 2\exp(-2K_1-2K_2) \end{aligned} \tag{8}$$

and from (5) and (7) after a simple transformation we have

$$\cosh(2K_1+2K_2)-\cosh(2K_1-2K_2)=4.25 \tag{9}$$

as an approximate critical condition for the $S=1$ model on the square lattice.

In the isotropic case $K_1=K_2=K$ our result $\exp(-K_c)=0.5568$ differs less than 1% from the best known numerical value, $\exp(-K_c)=0.5533$ (Burkhardt and Swendsen 1976).

The same procedure may be applied to other two-dimensional lattices for which in the case $S=\frac{1}{2}$ exact results were reproduced by the method of Hajduković and Šćepanović (1986). So, for example, the exact critical condition for an anisotropic honeycomb lattice was obtained by considering only a site of the lattice with its three neighbours. For such a system of four sites, the same rule as for the square lattice leads to $L=9$. Then, by starting with the exact critical condition for the $S=\frac{1}{2}$ model (Hajduković and Šćepanović 1986) a simple calculation yields:

$$\cosh(K_1+K_2+K_3)-\cosh(K_1+K_2-K_3)-\cosh(K_1-K_2+K_3)$$
$$-\cosh(-K_1+K_2+K_3)=2.25 \tag{10}$$

as an approximate critical condition for the $S=1$ model on the honeycomb lattice. In the isotropic case $K_1=K_2=K_3=K$ our result, $\exp(-K_c)=0.4285$, is in good agreement with the best known numerical value, $\exp(-K_c)=0.4217$ (Fox and Guttmann 1973).

In the case of a triangular lattice, extension of the critical condition for $S=\frac{1}{2}$ to the $S=1$ model gives

$$\exp(K_1+K_2+K_3)-\exp(K_1-K_2-K_3)-\exp(-K_1+K_2-K_3)$$
$$-\exp(-K_1-K_2+K_3)=1. \tag{11}$$

In the isotropic case we have $\exp(-K_c)=0.6884$ which is again in agreement with the numerical estimate, $\exp(-K_c)=0.6875$ (Fox and Guttmann 1973).

By starting with the critical condition for the $S=\frac{1}{2}$ model (Hajduković and Šćepanović 1986) the same procedure may be applied to the simple cubic lattice ($d=3$) with the spin $S=1$. The final result is

$$\cosh[2(K_1+K_2+K_3)]=\tfrac{81}{32} \tag{12}$$

and for the isotropic case $\exp(-K_c)=0.7684$. Comparison with the numerical estimate $\exp(-K_c)=0.7312$ (Fox and Guttmann 1973) shows that in the case $d=3$ the proposed approximation is not as good as in $d=2$ dimensions. This was to be expected because we started with critical conditions for $S=\frac{1}{2}$ which are exact in $d=2$ dimensions but only approximate in $d=3$ dimensions.

References

Burkhardt T W and Swendsen R H 1976 *Phys. Rev.* B **13** 3071
Fox P F and Guttmann A J 1973 *J. Phys. C: Solid State Phys.* **6** 913
Hajduković D 1983 *J. Phys. A: Math. Gen.* **16** L193
Hajduković D and Šćepanović R L 1986 *J. Phys. A: Math. Gen.* **19** L1015