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1983 J. Phys. A: Math. Gen. 16 L193

(http://iopscience.iop.org/0305-4470/16/6/004)

J. Phys. A: Math. Gen. **16** (1983) L193–L198. Printed in Great Britain

LETTER TO THE EDITOR

On the location of the critical point of the q-state Potts model on the hypercubic lattice

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Received 5 January 1983

Abstract. The critical temperature of the q-state ferromagnetic Potts model on a hypercubic lattice in d dimensions is expressed as an explicit function of both d and q. Our formula agrees very well with the existing accurate results and numerous numerical studies for particular values of d and q, and it seems to be an excellent approximation for all d and q.

The model considered in this paper is the q-state Potts ferromagnet on the hypercubic lattice in d dimensions (for a review see Wu 1982). To introduce the q-state Potts model we attach to every lattice site i a spin variable σ_i that takes values in the set $\{1, 2, \ldots, q\}$ and define the Hamiltonian by

$$\mathcal{H} = -\varepsilon \sum_{\langle ij \rangle} \delta_{kr}(\sigma_i, \sigma_j), \qquad \varepsilon > 0. \tag{1}$$

The sum is taken over pairs of nearest-neighbour sites $\langle ij \rangle$ and $\delta_{kr}(\alpha, \beta)$ is the Kronecker delta.

The exact critical point and the nature of the phase transition are known for the hypercubic lattice in $d = 2$ dimensions only (i.e. for the square lattice) (Potts 1952, Baxter 1973, Baxter *et al* 1978, Hintermann *et al* 1978). In this special case, the value of the critical coupling $K_c \equiv \varepsilon/kT_c$, where k is the Boltzmann constant and T_c is critical temperature, is a simple function of q:

$$K_c(d = 2, q) = \ln(1 + \sqrt{q}). \tag{2}$$

On the other hand, there is no exact result in three dimensions and the critical point can be located only by numerical means (Sykes *et al* 1972, Kim and Joseph 1975, Blöte and Swendsen 1979, Hermann 1979, Ditzian and Kadanoff 1979, Miyashita *et al* 1979, Ono and Ito 1982). For lattices in higher-than-three dimensions we are again guided by numerical studies only (Fisher and Gaunt 1964, Blöte and Swendsen 1979, Gaunt *et al* 1979, Ditzian and Kadanoff 1979). Table 1 lists the numerical estimates of the critical point obtained in these studies. In this situation, when we can only resort to numerical means, it is desirable to determine the critical coupling $K_c(d, q)$ as a function of the model characteristics d and q, as has been done in (2) for the particular case $d = 2$. In this paper we obtain such a general formula for $K_c(d, q)$. It is exact for $d = 1, 2$. The formula has not been obtained by a rigorous treatment and we cannot prove or disprove its validity for $d \geqslant 3$. However, as can be seen from table 1, our results for $d \geqslant 3$ are in excellent agreement with the numerical

Table 1. Numerical estimates of the critical point for the hypercubic lattice in d dimensions and results obtained by using formula (17).

q \ d		3	4	5	6	10
2	$e^{-K_c}=$	0.64816[a] 0.64469[j]	0.74100[b] 0.74132[c] 0.74292[j]	0.79607[b] 0.7979[j]	0.83134[b] 0.83341[j]	0.9018[j]
3		0.5784[d] 0.5769[f] 0.577[e] 0.571[g] 0.575[h] 0.5759[j]	0.6788[e] 0.6776[j]	0.7392[j]	0.7808[j]	0.8659[j]
4		0.523[g] 0.524[i] 0.532[h] 0.5319[j]	0.621[i] 0.6359[j]	0.678[i] 0.701[j]	0.721[i] 0.747[j]	0.821[i] 0.843[j]
6		0.472[h] 0.475[j]	0.5819[j]	0.652[j]	0.703[j]	0.812[j]

[a]Series analyses (Sykes *et al* 1972). [b]High-temperature series analysis (Fisher and Gaunt 1964). [c]High-temperature series analysis (Gaunt *et al* 1979). [d]Low-temperature series analysis (Miyashita *et al* 1979). [e]Monte Carlo renormalisation group (Blöte and Swendsen 1979). [f]Monte Carlo (Hermann 1979). [g]High-temperature series analysis (Kim and Joseph 1975). [h]Monte Carlo (Ono and Ito 1982). [i]High-temperature series analysis (Ditzian and Kadanoff 1979). [j]Results obtained by using formula (17).

studies. So, we expect our formula to be a very good approximation for *all d* and q. A discussion about this point will be given later.

The exact critical temperature (2) for a square lattice is the solution of

$$(e^K-1)^2=q. \tag{3}$$

Equation (3) was first obtained by Potts (1952) using the self-duality of the square lattice. We shall write this equation in an uncommon form

$$e^{2K}-2\,e^K-1=q-2, \tag{4}$$

which is convenient for the discussion which follows.

We will first obtain (4) for the particular case $q=2$, in an interesting but not rigorous manner, which will be of use later on as well. To this end we start with the Hamiltonian (1). Let us introduce a new variable, n, the number of terms for which $\delta_{kr}(\sigma_i,\sigma_j)=1$, into the Hamiltonian (1) which becomes

$$\mathscr{H}=-\varepsilon n. \tag{5}$$

The partition function is then

$$Z=\sum_n G(n)\,e^{Kn}\equiv\sum_n z(n). \tag{6}$$

Here $K\equiv\varepsilon/kT$, and the sum is taken over all possible values of n. $G(n)$ is the number of configurations with a given n, i.e. the degeneracy of the state with a fixed energy (5). It is very difficult to obtain $G(n)$, i.e. $z(n)$ for the entire lattice. They are, however, easily obtained for just a single square. The assumption is that the information about the critical temperature of the *infinite* system is retained in the values of

$z(n)$ for a *single* square. The possible values of n for a single square are $n = 0, 2, 4$ with energies $0, -2\varepsilon, -4\varepsilon$ and

$$z(0) = 2 \qquad z(2) = 12\,e^{2K} \qquad z(4) = 2\,e^{4K}. \tag{7}$$

The values of $n = 0, 2, 4$ can be classified into two groups. For $n = 0, 4$ the spin state of a spin uniquely determines the states of other spins on the square. For $n = 2$ the knowledge of the state of a single spin is not sufficient to determine the states of the others. In a way, $z(0)$ and $z(4)$ represent the states with rigorous regularity in order, while $z(2)$ represents the states with no regularity in order. Let us sum the $z(n)$, taking the $z(n)$ from one group with a minus sign and the $z(n)$ from the other group with a plus sign. Let us assume that at the critical temperature of an infinite lattice, the sum thus formed is equal to zero, i.e. that the critical temperature is the solution of

$$z(0) + z(4) - z(2) = 0. \tag{8}$$

If we introduce equation (7), equation (8) becomes

$$z(0) + z(4) - z(2) = 2(e^{4K} - 6e^{2K} + 1) = 2(e^{2K} - 2e^{K} - 1)(e^{2K} + 2e^{K} - 1) = 0,$$

i.e. because we are interested only in the solution with $K > 0$

$$e^{2K} - 2e^{K} - 1 = 0. \tag{9}$$

This equation is identical to (4) for $q = 2$ and its solution $K_c(d = 2, q = 2) = \ln(1 + \sqrt{2})$ is identical to the critical temperature obtained from the exact solution for $q = 2$ for the square lattice (Onsager 1944).

We do not know why the described procedure gives the exact result but it is obviously not a coincidence. The procedure also gives exact results for certain other lattices, e.g. the $q = 2$ triangular lattice, where if only a single triangle is considered, the possible values of n are $n = 3, 1$ with $z(3) = 2e^{3K}$ and $z(1) = 6e^{K}$. According to the rule described above, we form the equation $z(3) - z(1) = 0$ which gives the exact critical coupling $K_c = \ln\sqrt{3}$ (Wu 1982) for the $q = 2$ triangular lattice. (For other examples of the validity of the procedure see Švrakić (1980).) However, there are cases such as the honeycomb lattice where our procedure does not give satisfactory results. So, for a single hexagon, the possible values of n are $n = 6, 4, 2, 0$ with $z(6) = 2e^{6K}$, $z(4) = 30e^{4K}$, $z(2) = 30e^{2K}$, $z(0) = 2$. The exact critical coupling is the solution of the equation $z(6) + z(2) - z(4) - z(0) = 0$ (Wu 1982), whereas the procedure used for the square and triangular lattices would give $z(0) + z(6) - z(2) - z(4) = 0$. However, for all these equations which give the exact critical point, it is common that a linear combination of the $z(n)$ is equal to zero. We accept that it is true in the general case but we do not know an actual rule to obtain this linear combination. We now turn to the problem of the formation of the linear combination of the $z(n)$ for the hypercubic lattice.

Let us consider the general case of a lattice in d dimensions. The only equation we can start with is (4) for the special case of the $d = 2$ lattice. We note that the model characteristic q is a parameter in (4). Different values of the parameter give different values of critical temperature, but the structure of the equation does not change.

We will now make two crucial assumptions.

(i) The critical temperature is the solution of a general equation in which d and q, the model characteristics, are parameters. The general equation is of the same structure as (4) and for the particular case of $d=2$, it reduces to it.

A possible intuitive basis for this assumption is as follows. We are considering a hypercubic lattice in d dimensions in the d-dimensional Euclidean space. Its projection onto any subspace of the Euclidean space is also a hypercubic lattice in that *subspace*, i.e. the projection conserves the lattice type. Intuitively this could mean that the topological characteristics of the lattice that determine the critical temperature and the structure of the equation that give us this critical temperature are conserved also.

(ii) For very large q, if lower-order terms are neglected, the general equation reduces to $e^{dK}=q$, i.e. for very large q, to a good approximation $K_c(d,q)=\ln q^{1/d}$.

This assumption is the same as the mean-field theory result in the limit $q\to\infty$. In this limit the mean-field theory is exact (Pearce and Griffiths 1980, Wu 1982). Thus, our general equation will give the exact critical temperature for $d=2$ (i) and for all d in the limit $q\to\infty$ (ii).

According to our assumptions let us look for a general equation of the form

$$e^{dK}-a\,e^{dK/2}-b=q-2, \tag{10}$$

where a and b depend only on d and have to be determined. We shall first determine a and b for $q=2$ for a simple cubic lattice (hypercube in $d=3$ dimensions). We are going to use the quantities $z(n)$ as in the case of the square lattice. Let us consider a single cube. The possible values of n are $n=0$, 3, 4, 5, 6, 7, 8, 9, 12 with the corresponding

$$\begin{aligned} &z(0)=2 && z(3)=16e^{3K} && z(4)=30e^{4K}\\ &z(5)=48e^{5K} && z(6)=64e^{6K} && z(7)=48e^{7K}\\ &z(8)=30e^{8K} && z(9)=16e^{9K} && z(12)=2e^{12K}. \end{aligned} \tag{11}$$

As mentioned earlier, in the general case, we do not know how to form an equation from $z(n)$'s that would give the critical temperature. However, we wish to obtain (10) in which for $q=2$ and $d=3$ the only terms present are e^{3K}, $e^{3K/2}$, e^{0}. This is possible only if

$$z(3)+z(9)-z(6)=0 \tag{12}$$

which can be transformed into

$$16e^{3K}(e^{3K}-\sqrt{2}\,e^{3K/2}-1)(e^{3K}+\sqrt{2}\,e^{3K/2}-1)=0. \tag{13}$$

Thus, the critical temperature of the simple cubic, $q=2$, lattice is the solution of

$$e^{3K}-\sqrt{2}\,e^{3K/2}-1=0, \tag{14}$$

or, for a general value of q, according to (10)

$$e^{3K}-\sqrt{2}\,e^{3K/2}-1=q-2. \tag{15}$$

If we compare (4) and (15) for $d=2$, 3, we see that they are special cases of

$$e^{dK}-2^{1/(d-1)}\,e^{dK/2}-1=q-2. \tag{16}$$

Equation (16) satisfies our assumptions and we accept it for the general equation. As expected, the solution of this equation

$$K_c(d, q) = (2/d) \ln[\![\tfrac{1}{2}\{2^{1/(d-1)} + [4^{1/(d-1)} + 4(q-1)]^{1/2}\}]\!] \qquad (17)$$

gives the critical point of a hypercubic lattice for arbitrary d and q.

Of course, the procedure by which we obtained our principal results ((16) and (17)) is not rigorous. Expression (17) gives the exact critical coupling for $d=2$ and for $d \geqslant 3$ in the limit $q \to \infty$ since the formula was derived under these assumptions. It is, however, interesting that (17) is also exact for $d = 1$. Indeed,

$$\lim_{d \to 1} K_c(d, q) = \infty \qquad (18)$$

and it is the exact critical coupling for the one-dimensional ferromagnet. This supports formula (17). However, the principal support of (17) is the numerous numerical estimates, for different particular values of d and q. As given in table 1, there is excellent agreement between numerical studies and our results. For $q=2, 3$ the differences between them are less than 0.5%. For $q=4$, the differences are about 3% but these numerical values are less accurate and more careful analysis supports our results. Namely, for $q=4$, the estimates of critical temperatures were obtained from the high-temperature susceptibility series for dimensionality d (Ditzian and Kadanoff 1979). In the same paper the case of $q=4$, $d=4$ is considered more carefully. From the low-temperature susceptibility series they obtained the estimate $e^{-K_c}_{(L)} = 0.647$ which is slightly above the estimate $e^{-K_c}_{(H)} = 0.621$ from the high-temperature susceptibility. By using the free energy low- and high-temperature series they obtained $e^{-K_c} = 0.635$. The authors conclude: 'We think that the evidence is that at $d=4$ the $q=4$ Potts model undergoes a first-order phase transition at $e^{-K_c} = 0.635$ and that there are spinodal pseudo-transitions at $e^{-K_c}_{(H)} = 0.621$ and $e^{-K_c}_{(L)} = 0.647$'. As can be seen from table 1, the above analysis confirms our formula, i.e. the result $e^{-K_c} = 0.6359$ that is obtained from it in the considered case $q=4$, $d=4$. Let us emphasise another case in table 1, where both high- and low-temperature estimates have been given. This is for $q=3$, $d=3$ and our estimate lies between the two.

Thus both the exact values and numerical estimates confirm formula (17) and indicate that it gives a good approximation for the critical temperature for *all* d and q. The possibility that (17) is exact for some other cases besides $d = 1, 2$ also cannot be completely excluded. We hope that further study of (16) will ensue. Further numerical investigations for larger q are welcome. Even more important would be an understanding of the theoretical basis that might lead to (16). In this respect, our intuitive approach leaves a lot of questions to be answered.

I would like to thank the staff of CERN Theoretical Division, T Faberge, M Fontaine, M O'Halloran and A Perrin, whose enthusiasm and kind help are known to everyone who spent some time at CERN. I also acknowledge stimulating discussions with Professors H Capel and S Milošević.

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