Journal of the Korean Physical Society, Vol. 15, No. 2, September, 1982

Large q expansion of the Potts Model Susceptibility and Magnetization in Two and Three Dimensions*

Hyunggyu Park and Doochul Kim

Department of Physics, Seoul National University, Seoul, .51, Korea

(Received 18 June, 1982)

The large q expansion formalism of the q state Potts model is used to obtain the susceptibility and the spontaneous magnetization series at the first order phase transition temperature for two and three dimensional lattices. The series analysis in three dimensions does not reveal any definite information as to singularity structure at the critical value of q where the transition becomes continuous.

Accurate estimates of the transition temperatures of three dimensional lattices for $q>3$ are obtained.

I. INTRODUCTION

The q-state Potts model[1], a generalization of the Ising model, is a lattice spin model in which the number of states each spin on a lattice site can take is an integral number q while the interaction energies between nearest-neighbor spin pairs depend only on whether the two spins are in the same state or not. The model can be used to describe various physical situations[1] such as percolation problems, the order-disorder phase transitions of adsorbed ^{4}He monolyers on substrates, and certain magnetic transitions with a special symmetry. An interesting feature of the model is that, for two dimensional lattices, the phase transition is continuous for $q<q_c = 4$ while it is discontinuous for $q>q_c$[2,3]. The mechanism for the occurrence of the critical value of q_c which divides the continous and discontinuous phase transitions has been elucidated by Nienhuis et al.[4,5] by considering a Potts lattice gas using position-space renormalization-group transformations. On the basis of this, Cardy et al.[6] have constructed a scaling theory near q_c which predicts that the latent heat, the discontinuity of the magnetization and the inverse susceptibilities at the transition temperature T_c all vanish as $q \to q_c^+$, with an essential singularity in $(q-q_c)^{1/2}$.

On the other hand, when $q \to \infty$, the mean field theory becomes exact provided the temperature variable is appropriately scaled, and this allows one to construct systematic expansions for the free energy in power series of $q^{-2/z}$ where z is the coordination number of the lattice[7,8]. One of us[7] investigated the large q expansions of the magnetization discontinuity, ΔM, for two dimensional lattices and found that they are independent of the lattice structures. Shortly afterward, Baxter[9] showed that this is a consequence of the duality properties of the planar Potts model and further produced an exact expressions for ΔM using his corner transfer matrix approach. His result is consistent with the scaling picture of Cardy et al.

In three dimensions, no exact results are known. There is some weak evidence that the three state

* This work is supported by the Research Institute for Basic Sciences, Seoul National University.

Potts model in three dimensions exhibits a first order phase transition, which implies $2<q_c<3$.[10,11,12,13] More recently, Nienhuis et al.[14] have strongly argued that $q_c \sim 2.2$, assuming that the singularity structure in three dimensions is the same as that in two dimensions. Kogut and Sinclair [8] have obtained a latent heat series for the simple cubic lattice by the large q expansion method and have concluded that the latent heat has a power law singularity as $q \to q_c^+$ with $q_c \sim 2.6$. They also considered the Hamiltonian version of the Potts model leading to a suggested $q_c = 2.6 \sim 2.8$.[15]

In this work, we report calculation of large q expansions of the susceptibility (χ^-) and the spontaneous magnetization (ΔM) evaluated at the ordered side of the first order transition temperature T_c for various lattices. For the simple, body-centered and face-centered cubic lattices, we obtain ΔM and χ^- to $0(q^{-4})$ while for the square and triangular lattices we obtain χ^- to $0(q^{-5})$. The series for the critical temperatures of three dimensional lattices and for χ^+, the susceptibility of two dimensional lattices evaluated at the disordered side, are also obtained. Since the general methods appear elsewhere, we briefly discuss the method to set the notations and list our new results in section II. In section III, we discuss our analysis of the series. Unlike other series expansion methods, the large q expansions are found to be very poor in convergence and are not instrumental in predicting, with the presently available series, the singularity structures of the thermodynamic quantities.

However, we are able to determine the critical temperatures of three dimensional lattices rather accurately for all $q \gtrsim 3$. Other conclusions drawn from the series are also discussed in section III.

II. LARGE q EXPANSION

The Potts hamiltonian with N spins is given by

$$-\beta H = K \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j} + h \sum_{i=1}^{N} \delta_{\sigma_i, 1} \qquad (1)$$

where σ_i is the spin variable at lattice site i and takes q integer values (1,2, . . . , q), δ denotes the Kronecker delta function, K and h are the interaction and the symmetry breaking magnetic field, and the first sum is over the nearest neighbor pairs. The high temperature expansion of the zero field partition function (Z^+) is given by [16]

$$Z^+ = q^N (1+u/q)^{zN/2} \left\{ 1+\sum_G W(G) \left(\frac{u}{u+q}\right)^{\ell_G} \right\} \qquad (2)$$

where z is the coordination number, $u=e^K-1$, the sum is over the closed subgraphs, ℓ_G is the number of lines in a given graph G, and W(G) is 1/q times the number of ways one can color the lattice with q colors in such a way that the boundary lines where different colors meet coincide with the lines of G. Since $u \sim 0(q^{2/z})$ at the transition temperature [7], only small size graphs contribute to equation (2) for a given order of $q^{-2/z}$ and this enables one to develop systematic expansions in $q^{-2/z}$. The low temperature expansion of the partition function (Z^-) is discussed in reference [7]. In three dimensions the transition temperatures are obtained by matching the high and low temperature zero field free energy expressions order by order in fractional powers of $1/q$[8].

The order parameter of the ferromagnetic Potts model is the spontaneous magnetization given by

$$M = \lim_{h\to 0} \lim_{N\to\infty} \left(q \frac{\partial}{\partial h} N^{-1} \ln Z^- - 1\right)/(q-1). \qquad (3)$$

The magnetization discontinuity (ΔM) at the transition temperature is defined as

$$\Delta M = M(K)\,|_{K=K_c} \tag{4}$$

where K_c is the transition temperature. The high and low temperature susceptibilities at the transition temperature ($\chi^{\pm}$) are defined as

$$\chi^{\pm} = \lim_{h\to 0} \lim_{N\to\infty} \frac{\partial}{\partial h}\left(q\frac{\partial}{\partial h} N^{-1} \ln Z^{\pm} - 1\right)/(q-1)_{K=K_c}. \tag{5}$$

The latent heat (L) is given by

$$L = U^{+} - U^{-} = \left(\frac{\partial \ln Z^{+}}{\partial(-\beta)}\right) - \left(\frac{\partial \ln Z^{-}}{\partial(-\beta)}\right)|_{K=K_c}. \tag{6}$$

where $U^{\pm}$ are the internal energy at the transition temperature for the disordered and ordered phases respectively.

The results of our calculations are as follows. For the simple cubic (SC) lattice, we find that

$$\exp(-K_c) = x_1\left(1 - x_1^2 + \frac{4}{3}x_1^3 - 3x_1^5 + \frac{59}{9}x_1^6 - 6x_1^7 - 10x_1^8 + \frac{4298}{81}x_1^9 + \cdots\right), \tag{7}$$

$$\Delta M_{SC} = 1 - x_1^3 - x_1^6 - 6x_1^8 + 23x_1^9 - 38x_1^{10} + 8x_1^{11} + 217x_1^{12} + \cdots, \tag{8}$$

and

$$\chi_{SC}^{-} = q^{-1}\left(1 + 6x_1^2 + 30x_1^4 - 14x_1^5 + 6x_1^6 + 168x_1^7 - \frac{440}{3}x_1^8 - 56x_1^9 + \cdots\right) \tag{9}$$

where $x_1 = q^{-1/3}$. For the face-centered cubic (FCC) lattice, the results are

$$\exp(-K_c) = x_2\left(1 - x_2^5 + \frac{7}{6}x_2^6 - \frac{4}{3}x_1^9 + 4x_2^{10} - 6x_2^{11} + \frac{235}{72}x_2^{12} - 4x_2^{13} + \frac{39}{2}x_2^{14} - \frac{326}{9}x_2^{15} + \frac{97}{3}x_2^{16} - 30x_2^{17} + \frac{89713}{1296}x_2^{18} + \cdots\right), \tag{10}$$

$$\Delta M_{FCC} = 1 - x_2^6 - x_2^{12} - 8x_2^{15} + 24x_2^{16} - 24x_2^{17} + 3x_2^{18} - 48x_2^{19} + 186x_2^{20} - 180x_2^{21} - 122x_2^{22} + 28x_2^{23} + 1765\ x_2^{24} + \cdots, \tag{11}$$

and

$$\chi_{FCC}^{-} = q^{-1}\left(1 + 12x_2^5 - 12x_2^6 + 56x_2^9 - 36x_2^{10} - 86x_2^{11} + 92x_2^{12} + 336x_2^{13} - 518x_2^{14} - 472x_2^{15} + 1638x_2^{16} + \frac{4687}{6}x_2^{17} - 5916x_2^{18} + \cdots\right) \tag{12}$$

where $x_2 = q^{-1/6}$; while for the body-centered cubic (BCC) lattice, the series are

$$\exp(-K_c) = x_3\left(1 - x_3^3 + \frac{5}{4}x_3^4 - 2x_3^7 - \frac{19}{32}x_3^8 + 12x_3^9 - 21x_3^{10} + 26x_3^{11} - \frac{8029}{128}x_3^{12} + \cdots\right), \tag{13}$$

$$\Delta M_{BCC} = 1 - x_3^4 - x_3^8 - 25x_3^{12} + 96x_3^{13} - 180x_3^{14} + 216x_3^{15} - 217x_3^{16} + \cdots, \tag{14}$$

and

$$\chi_{BCC} = q^{-1}\left(1 + 8x_3^3 - 8x_3^4 + 56x_3^6 - 106x_3^7 + 216x_3^8 - 280x_3^9 + 200x_3^{10} + \frac{2757}{4}x_3^{11} - 2614x_3^{12} + \cdots\right) \tag{15}$$

where $x_3 = q^{-1/4}$. In the above, ΔM_{SC} denotes ΔM of the SC lattice, etc. The latent heat series for the simple cubic lattice has been obtained by Kogut and Sinclair.[8] Here, we find the latent heat series for the face-centered cubic lattice to be

$$L = \left(1 - x_2^5 - 2x_2^6 - 4x_2^9 + 8x_2^{10} - \frac{17}{6}x_2^{11} - 2x_2^{12} - 20x_2^{13} + \frac{242}{3}x_2^{14} - 116x_2^{15} + \frac{172}{3}x_2^{16} - \frac{5863}{72}x_2^{17} + 394x_2^{18} + \cdots\right)/6J \tag{16}$$

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where $\beta J = K$. The latent heat series for the body-centered cubic lattice can be easily calculated and is not shown here.

In two dimensions, ΔM, L and K_c are known exactly for all q.[2,3,9,17] The susceptibilities at K_c, $\chi^{\pm}$, are found to be

$$\chi^-_{SQ} = q^{-1}(1+4z_1 + 22z_1^2 + 76z_1^3 + 304z_1^4 + 968z_1^5 + 3322z_1^6 + 9972z_1^7 + 31253z_1^8 + \cdots), \quad (17)$$

$$\chi^+_{SQ} = q^{-1}(1+4z_1 + 20z_1^2 + 68z_1^3 + 268z_1^4 + \cdots\cdot), \quad (18)$$

$$\chi^-_{TR} = q^{-1}(1+6z_2^2 + 8z_2^3 + 30z_2^4 + 56z_2^5 + 166z_2^6 + 320z_2^7 + \frac{2332}{3}z_2^8 + 1674z_2^9 + \frac{10682}{3}z_2^{10} + \frac{203356}{27}z_2^{11} + 15961z_2^{12} + \cdots), \quad (19)$$

and

$$\chi^+_{TR} = q^{-1}(1+6z_2^2 + 6z_2^3 + 30z_2^4 + 44z_2^5 + 156z_2^6 + \cdots\cdot\cdot) \quad (20)$$

where SQ and TR denote the square and triangular lattices, $z_1 = q^{-1/2}$ and $z_2 = q^{-1/3}$, respectively.

III. DISCUSSION

We have analyzed the series eqs. (7) – (20) by constructing various kinds of Padé approximants [18] in the hope that they would reveal singularity structures near q_c. In two dimensions, the latent heat and the magnetization discontinuity behave as follows as $q \to 4^+$,

$$L \sim \exp(-\frac{1}{2}\pi^2(q-4)^{-1/2}), \quad (21)$$

and

$$\Delta M \sim \exp(-\frac{1}{8}\pi^2(q-4)^{-1/2}). \quad (22)$$

Using Cardy et al. 's phenomenological theory, we find the behavior of $\chi^{\pm}$ to be

$$\chi^{\pm} \sim \exp(\frac{7}{4}\pi^2(q-4)^{-1/2}). \quad (23)$$

To see if the series bear out the asymptotic form given by eq. (23), we have investigated Padé approximants to d ln χ^-/dz (Dlog), d ln(d ln χ^-/dz)/dz (Dlog Dlog), d ln (ln χ^-)/dz (Dlog log) and (ln $\chi^-)^2$ (ln ^{2}) for the $\chi^-(z)$ series given by eqs. (17) and (19) where $z = z_1$ or z_2. If the asymptotic behavior of the series is given by eq. (23), the Dlog Dlog, Dlog log and ln^2 Padés should have a simple pole near $z = z_c$ where $z_c = 4^{-1/2}$ for eq. (17) and $4^{-1/3}$ for eq. (19)[19]. The various Padé tables we have obtained do not show any consistent location for the poles indicating that the series we have are not long enough to probe the asymptotic region near $q \simeq q_c$. The Dlog log Padé shows a few poles near q_c with residues of ~ 0.5 which is expected for a singularity of the form of eq. (23), but the data are not good enough to enable one to draw any confident conclusions. On the other hand, the Dlog Padés show slightly better consistency for the location of the poles but here the residues associated with the physical poles are rather large (~7.8) indicating a stronger singularity than the usual algebraic one.

The series for the three dimesional lattices have more terms than those for the two dimensional ones, but in powers of q^{-1} they go up only to lower orders. Therefore we would expect the series to reflect information around q_c no better than the two dimensional ones. The Dlog Padés of the χ^- series give a few poles around $q_c \simeq 2.5 \sim 3.0$ with residues of 2.5 ~ 3.0. This behavior is also found by Kogut and Sinclair[8] in their analysis of the simple cubic lattice latent heat. This data supports

Table I. Critical temperatures of the q-state Potts model for the simple, face-centered and body-centered cubic lattices obtained from the large-q expansion method. The values of $\exp(-K_c)$ are listed.

Lattice \ q	2	3	4	5	6
S.C.	.641±.008	.575±.003	.532±.001	.501±.001	.4771±.0004
F.C.C.	.813±.003	.771±.001	.7420±.0005	.7196±.0002	.7018±.0002
B.C.C.	.732±.008	.673±.006	.634±.003	.606±.001	.583±.001

the conclusion of Kogut and Sinclair who preferred the algebraic singularity. However, this behavior is also observed in the two dimensional cases where the essential singularity is expected. Furthermore, in the Dlog log Padés for the χ^- and L series, we find a few poles around $q_c \simeq 2.0\sim2.3$ with residues of ~ 0.5, similar to that for two dimensions. Results from other Padés are no more illuminating. In short, from the series we have at hand, we are not able to discern whether the behaviors of ΔM, L or χ near q_c are of the algebraic or essential type.

As can be seen in eqs. (8), (11) and (14), ΔM is lattice-dependent in three dimensions in contrast to the lattice independent result for two dimensions. Also the amplitude ratios of the susceptibilities at T_c (χ^+/χ^-) are lattice-dependent. This suggests that the "universal" behavior of ΔM in two dimensions is a special property due to the duality relations and not a general feature of the model. In the renormalization group context, the first order phase transition is associated with the first order fixed points of the renormalization group transformations.[20]
The non-universal behaviors of ΔM, L, and $\chi^\pm$ imply that they are not local properties of the first order fixed point.

Accurate determination of the critical temperatures of the three dimensional Potts model is useful in checking the reliability of other approximate methods. We find that the direct Padé approximants to the series, eqs. (7), (10) and (13), give accurate estimates of the critical value $\exp(-K_c)$ down to $q\simeq3$. The values we obtained are listed in Table I for the three lattices for q = 2,3, 4,5, and 6. As the series is an expansion around $q=\infty$, our estimates are better for larger q. Although the series loses its meaning below q_c, the approximants evaluated even at q=2 give good agreement with the Ising model data.[21] Also, we see that the critical temperatures determined from the high temperature expansion method[10] are lower than our values and those from the low temperature expansion method[11] are higher. For example, for the simple cubic lattice, with q=3, the high temperature series gives $\exp(-K_c)\simeq 0.571$ and the low temperature series gives $\exp(-K_c) \simeq 0.578$ while our result is $\exp(-K_c) \simeq 0.575$. This is quite reasonable since the estimates from those expansion methods tend to overshoot the first order phase transition point. Recent data obtained by Ono and Ito[22] from Monte Carlo simulations are in excellent agreement with our result. They find, for the simple cubic lattice, $\exp(-K_c)\simeq 0.575$, 0.532 and 0.472 for q=3, 4 and 6, respectively.

ACKNOWLEDGEMENT

We are grateful to Messrs. Kiho Kang, Hyungtae Kuk, and Seung-hwan Kim at Seoul National University for participating in the early stage of this work and checking some of our series coefficients.

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