High-temperature series study of the q-component Potts model in two and three dimensions

1975 J. Phys. A: Math. Gen. 8 891

(http://iopscience.iop.org/0305-4470/8/6/008)

J. Phys. A: Math. Gen., Vol. 8, No. 6, 1975. Printed in Great Britain.

High-temperature series study of the q-component Potts model in two and three dimensions

D Kim† and R I Joseph‡

† Physics Department, New York University, New York, New York 10003, USA
‡ Department of Electrical Engineering, The Johns Hopkins University, Baltimore, Maryland 21218, USA

Received 15 October 1974, in final form 19 December 1974

Abstract. High-temperature series for the free energy of the q-component Potts model in the presence of arbitrary external fields are generated to eighth order for five lattices and subsequently analysed. In two dimensions the higher critical exponents γ, γ_3 are estimated to be 1·42, 3·60 and 1·20, 2·62 for $q = 3$ and 4 respectively. Evidence for the possible divergence of the order parameter fluctuation at the first-order transition point for $q \geqslant 5$ is presented. In three dimensions the question of the order of the transition is directly investigated in the temperature–order parameter plane and analysis of the series indicates that the transition is of first order for $q \geqslant 3$.

1. Introduction

Recently there has been considerable interest in the statistics of the Potts model (Potts 1952). For this model a spin at the ith lattice site σ_i can take on the q values $1, 2, \ldots, q$. The interaction energy between nearest-neighbour pairs is $-J$ if they are in the same state and zero otherwise.

Apart from its purely theoretical interest in statistical mechanical problems, the Potts model is now emerging as a serious candidate to describe various physical situations. Recently Alexander and Yuval (1974) discussed the relevance of this model to a situation where the order parameter is a second-rank tensor, such as in the isotropic-to-nematic liquid crystal phase transition or plastic transitions in molecular crystals. Priest (1971) also considered this Potts interaction as a quantized version of the rotationally invariant potential in the lattice model of nematic liquid crystals.

In two dimensions Potts (1952) used the transfer matrix approach to find the inversion transformation for a square lattice and thus was able to locate the transition temperatures for all q. Kihara *et al* (1954) proposed the same model independently in connection with the solid–liquid transition and found the Onsager-type dual transformation by a topological approach. Mittag and Stephen (1971) also studied the dual transformation on the square lattice. More recently Kim and Joseph (1974a) located the exact transition temperatures on the triangular and honeycomb lattices for all q using a generalized star–triangle transformation by introducing a three-spin interaction.

An important result was recently obtained by Baxter (1973) who has shown that on a square lattice this model has a non-vanishing latent heat only for $q > 4$. This result strongly implies that other first derivatives of the free energy are also continuous at the transition for $q \leqslant 4$. A continuous transition for $q \leqslant 4$, in any sense, is contrary to the

prediction of the mean field approximation (MFA). The MFA and equivalent phenomenological arguments predict that the transition is of first order (discontinuous) for $q > 2$ in all dimensions. In fact the validity of the MFA for $q = 3$ in two dimensions had previously been questioned by a number of workers on the basis of series expansion work on the square lattice (Straley and Fisher 1973, Kihara *et al* 1954). On the other hand the ϵ-expansion work of Amit and Shcherbakov (1974) in the four-dimensional limit supported the idea of a first-order transition for $q = 3$.

Consequently a question of considerable interest is whether in three dimensions the Potts model exhibits a first-order phase transition (in zero fields), as the MFA predicts, or a continuous transition for lower q's as in two dimensions. There are a number of previous studies relevant to this question for $q = 3$. One is that of Golner (1973) who studied a continuum generalization of the $q = 3$ Potts model by means of Wilson's $\eta = 0$ approximate renormalization group recursion formula. Another is that of Ditzian and Oitmaa (1974) in which the spin 1 Ising Hamiltonian with biquadratic interactions was studied by means of a six-term high-temperature susceptibility series for the face-centred cubic lattice for a range of biquadratic interactions which included the Potts model. Lastly, low- and high-temperature series of various thermodynamic quantities were constructed and analysed by Straley (1974) for the simple cubic lattice and by Enting (1974) for the face-centred cubic lattice. The authors of the first two works preferred to interpret their results as evidence for a first-order transition while the last two authors interpreted their own results as evidence for a second-order transition. None of these works, however, is by any means conclusive in its results.

In our work we have approached this problem from a different point of view. Unlike conventional approaches, derivatives of the free energy as a function of an order parameter m (not a field) and the temperature are investigated directly in the m–T plane. The criterion used to distinguish between a continuous and a discontinuous transition is that in the latter case the susceptibility should diverge for a finite value of m at a temperature higher than the transition temperature. Detailed arguments concerning this point are given in § 4. Analysis of our high-temperature series (§ 2) in this context gives good evidence for a discontinuous transition in m for $q \geqslant 3$ for all three-dimensional lattices considered. The high-temperature series obtained are also utilised to estimate the critical point exponents associated with higher-order critical points in two dimensions, where the transition is known to be continuous. We also present evidence of possible diverging fluctuations at the first-order transition (§ 3). In § 5 scaling relations and the relevance of the Potts model to liquid crystals are discussed.

2. High-temperature series expansion of the free energy in a field

The Hamiltonian of the system may be written as

$$-\beta\mathscr{H} = K \sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j} + \sum_{i=1}^{N} \zeta(\sigma_i) \tag{1}$$

where $K = \beta J$ and $\zeta(\sigma_i) = \zeta_k$ when $\sigma_i = k$. Here the ζ_k are symmetry breaking fields. If we let n_k be the fraction of spins in the kth state, it is obvious that

$$\sum_{i=1}^{N} \zeta(\sigma_i) = N \sum_{k=1}^{q} \zeta_k n_k \tag{2}$$

and ζ_k becomes the field conjugate to the density $\langle n_k \rangle$, $\langle\ \rangle$ denoting a thermal average. Because of the condition

$$\sum_{k=1}^{q} n_k = 1, \tag{3}$$

one of the ζ_k is irrelevant.

For specific zero field quantities, such as the susceptibility or free energy at $\zeta_k = 0$ for all k, a formalism for series generation has been previously developed by several authors (Mittag and Stephen 1971, Kihara *et al* 1954, Alexander and Yuval 1974). For the purpose of this study, however, it is necessary to include the arbitrary fields exactly.

Using the relation $\exp(K\delta_{\sigma\sigma'}) = 1 + [\exp(K) - 1]\delta_{\sigma\sigma'}$, the partition function can be written as

$$Z_N = \mathrm{Tr}\ \exp\left(\sum_{i=1}^{N} \zeta(\sigma_i)\right) \prod_{\langle ij \rangle} (1 + u\delta_{\sigma_i\sigma_j}) \tag{4}$$

where $u \equiv \exp(K) - 1$. Thus we can generate power series for the free energy f in the variable u.

At this stage it is convenient to define a set of functions:

$$G_n \equiv g_n / g_1^n \tag{5}$$

$$g_n \equiv \sum_{k=1}^{q} \exp(n\zeta_k). \tag{6}$$

Then all of the field and q dependences in the final results will be explicitly contained in the G_n functions. In the expansion of equation (4) the first term is g_1^N and each l line graph which can be drawn on a lattice contributes to the lth power in u with a factor determined by the topology of the graph. If we factor out g_1^N, an m-vertices connected graph gives a factor G_m so that each coefficient of u^l will be a linear combination of terms of the form $G_2^{\alpha_2} G_3^{\alpha_3} \ldots$. Thus we see that the free energy takes the form, after going to the thermodynamic limit,

$$-\beta f = \ln g_1 + \frac{z}{2} G_2 u + \left(\frac{z}{2}(z-1)G_3 - \frac{z}{2}(z-\tfrac{1}{2})G_2^2\right)u^2 + \ldots \tag{7}$$

where z is the lattice coordination number.

In our calculations we used the finite cluster method (Domb 1960), exploiting the data compilation of Baker *et al* (1967). The entire calculation was computerized and careful internal checking was performed. Overall checking was done by reducing the results to those known for the Ising model. In this way we obtained the free energy series through u^8 for the plane square (SQ), triangular (TR), simple cubic (SC), body-centred cubic (BCC) and face-centred cubic (FCC) lattices. The numbers of different terms for the lth power in u for FCC for example were 1, 2, 4, 7, 12, 21, 32, 50 for $l = 1, \ldots, 8$ respectively.

For our purpose it is sufficient to consider the situation where $\zeta_2 = \zeta_3 = \ldots = 0$. Then the G_n functions can be represented as power series of order n in a field variable τ defined by

$$\tau \equiv \frac{\exp(\zeta_1) - 1}{\exp(\zeta_1) + r} \tag{8}$$

where $r \equiv q-1$, ie

$$G_n(\zeta_1, 0, 0, \ldots) = q^{1-n} \sum_{k=0}^{n} \binom{n}{k} \left(\frac{r^k + (-1)^k r}{q}\right) \tau^k. \tag{9}$$

The order parameters of interest are the particle densities $\langle n_k \rangle$. The $\langle n_k \rangle$ are not independent and it is sufficient to consider only $\langle n_1 \rangle$ (Kim and Joseph 1974b). Hence we define a generalized 'magnetization':

$$m \equiv r^{-1}(q\langle n_1 \rangle - 1) = r^{-1}[q\partial(-\beta f)/\partial\zeta_1 - 1] \tag{10}$$

so that as $\zeta_1 \to 0^+$, $\zeta_2 = \zeta_3 = \ldots = 0$, the spontaneous ordering varies from zero at high temperatures to 1 at $T = 0$. The magnetization series for each q hence takes the form:

$$m = \tau \sum_{n=0}^{\infty} v^n \sum_{k=0}^{2n} a_{n,k}\tau^k = \phi_1(v)\tau + \phi_2(v)\tau^2 + \ldots \tag{11}$$

where we have changed to a new high-temperature variable,

$$v \equiv \frac{\exp(K)-1}{\exp(K)+r} = \frac{u}{u+q}. \tag{12}$$

In order to investigate the phase boundary, it is necessary to invert the series equation (11) to the form:

$$\tau = m \sum_{n=0}^{\infty} v^n \psi_n(m) \tag{13}$$

where

$$\psi_n(m) = \sum_{k=0}^{2n} b_{n,k} m^k. \tag{14}$$

We have confirmed that our results reduce to those of Gaunt and Baker (1970) for the $q = 2$ Ising case. Since the coefficients in either equation (11) or equation (14) are obtained for each q and for each lattice from a free energy result of the form equation (7), we present here only those series used in § 3 for the two-dimensional lattices (appendixes A.1 and A.2), and (appendix A.3) the $\psi_n(m)$ polynomial for the $q = 3$ FCC lattice used in § 4. All other series are available on request.

3. Analysis of series in two dimensions

As mentioned in the introduction, Baxter (1973) has rigorously shown that the Potts model in zero field undergoes a continuous transition for $q = 3$ and 4 on the square lattice in the sense that $\partial f/\partial T$ is continuous at the transition temperature. We shall assume that the order of the transition does not depend on which density (first derivative of the free energy with respect to a field) we are looking at; that is, we will assume that the continuity or discontinuity of $\partial f/\partial T$ is the same as that of $\partial f/\partial\zeta_1$. This is a reasonable assumption except for an accidental choice of the direction of the fields. Also, we shall assume that the nature of the transition is insensitive to the lattice structure in a given dimension, so that the spontaneous magnetization is also continuous for the triangular lattice for $q \leqslant 4$ and discontinuous for $q > 4$.

Because of the basic symmetry with respect to the fields (Kim and Joseph 1974b), a continuous transition in zero fields implies that the transition points must be critical points of higher order in the sense of Chang *et al* (1973). For $q = 3$ three lines of critical points meet at the transition; hence it is the tricritical point (Straley and Fisher 1973). For $q = 4$, by the same reasoning as in Straley and Fisher (1973), the transition point is a critical point of order four. For the $q = 2$ Ising case the free energy is an even function of the magnetic field. Hence the high-temperature gap exponents Δ_l are defined only for l even. But for the Potts model ($q \geqslant 3$) there is no longer such a symmetry and we can accordingly define a 'first gap exponent', $\Delta_1 \equiv \gamma_3 - \gamma$, as

$$\partial^2 m/\partial \zeta_1^2 \equiv \chi_3 \sim (v_0 - v)^{-\gamma-\Delta_1} \sim (v_0 - v)^{-\gamma_3}, \tag{15}$$

associated with the critical point of higher order.

In terms of the $\phi_i(v)$ polynomials of equation (11) we see that

$$\chi = \partial m/\partial \zeta_1 = q^{-1}(1-\tau)(1+r\tau)\,\partial m/\partial \tau|_{\tau=0} = \phi_1/q \tag{16}$$

and similarly,

$$\chi_3 = q^{-2}[(q-2)\phi_1 + 2\phi_2]. \tag{17}$$

The series for χ and χ_3 derived in this way are tabulated in appendixes A.1 and A.2 respectively for the TR and SQ lattices together with those for higher q's which are also used in this section.

These series were studied by standard methods of series analysis. For $q = 3$ and 4 the agreement of the poles of the Padé approximants (PA) to $\mathrm{d}(\ln \chi)/\mathrm{d}v\,(D \lg \chi)$ and $\mathrm{d}(\ln \chi_3)/\mathrm{d}v\,(D \lg \chi_3)$ with the exactly known transition temperatures were good enough to support the power law behaviour assumption. γ and γ_3 were estimated by constructing Padé approximants to $(v_0 - v)\,\mathrm{d}(\ln \chi)/\mathrm{d}v$ and $(v_0 - v)\,\mathrm{d}(\ln \chi_3)/\mathrm{d}v$ respectively for both the SQ and TR lattices. The estimated exponents are

$$q = 3: \gamma = 1{\cdot}42 \pm 0{\cdot}05$$
$$\gamma_3 = 3{\cdot}00 \pm 0{\cdot}1,$$

and

$$q = 4: \gamma = 1{\cdot}20 \pm 0{\cdot}05$$
$$\gamma_3 = 2{\cdot}62 \pm 0{\cdot}1$$

for both lattices. The confidence limits are determined by ratio methods and are considered to be conservative.

For $q > 4$ we have first-order transitions. In the mean field approximation the first-order transition occurs mathematically by choosing the lowest energy solution to the equation of state. This results in a finite susceptibility at the transition. Therefore, the high- and low-temperature susceptibilities in the MFA diverge at a temperature far beyond the transition temperature. On the high-temperature side, in the MFA we have

$$\left.\frac{\mathrm{d}\zeta_1}{\mathrm{d}m}\right|_{m=0} = q - \left(\frac{zJ}{k_B T}\right) \tag{18}$$

for

$$\frac{zJ}{k_B T} \leqslant \frac{2(q-1)\ln(q-1)}{q-2}, \tag{19}$$

ie $\chi \sim (T-T_c^*)^{-1}$, while the transition occurs at a temperature T_0 which is larger than T_c^*. For example, with $z = 6$, $v_0 = 0{\cdot}1456$ and $v_c^* = 0{\cdot}2065$ for $q = 5$ and $v_0 = 0{\cdot}1374$ and $v_c^* = 0{\cdot}2226$ for $q = 6$, in terms of the variable v.

Whether or not this feature will persist in an 'exact' calculation is an interesting question which needs further study. If we assume that $\chi \sim (v_c^* - v)^{-\lambda}$ etc we can estimate v_c^* by constructing Padé approximants to the logarithmic derivatives of the χ series. In table 1 we list the location of the physical poles for the six most significant approximants for $q = 5, 6$ for χ and also for the χ_3 series for the square lattice. In table 2 we list those for the triangular lattice where we have also included the $[2, M]$ Padé approximants as well as results for the $q = 7$ and 8 χ series. The agreement of the poles and the exact transition temperatures v_0 are surprisingly good for all cases shown, even for higher q. The poles of χ seem to give slightly higher estimates for v_0. This may be due to the effect of the mean-field-like trend of the first few terms. The reasonable regularity of the distribution of the poles supports the power law assumption. Hence we can

Table 1. Physical poles of the PA to $D \lg \chi$ and $D \lg \chi_3$ for $q = 5, 6$ for the SQ lattice.

Approximant	$q = 5$ ($v_0 = 0{\cdot}3090$)		$q = 6$ ($v_0 = 0{\cdot}2899$)	
	χ	χ_3	χ	χ_3
[5, 2]	0·3236	0·3051	0·3055	0·2738
[4, 3]	0·3104	0·3090	0·2923	0·2916
[3, 4]	0·3104	0·3059	0·2923	0·2870
[4, 2]	0·3396	0·3099	no pole	0·2972
[3, 3]	0·3102	0·3098	0·2921	0·2953
[3, 2]	0·2945	0·3088	0·2762	0·2885

Table 2. Physical poles of the PA to $D \lg \chi$ for $q = 5, 6, 7, 8$ and to $D \lg \chi_3$ for $q = 5, 6$ for the TR lattice. An asterisk denotes a smaller positive real pole with extremely small residue which is ignored.

Approximant	$q = 5$ ($v_0 = 0{\cdot}1808$)		$q = 6$ ($v_0 = 0{\cdot}1662$)	
	χ	χ_3	χ	χ_3
[5, 2]	0·1910*	0·1636	0·1725*	0·1687*
[4, 3]	0·1837*	0·1806	0·1692*	0·1688*
[3, 4]	0·1820	0·1736	0·1679	0·1682*
[2, 5]	0·1804	0·1802	0·1667	0·1656
[4, 2]	0·1821	0·1815	0·1691	0·1683
[3, 3]	0·1825	0·1813	0·1691	0·1678
[2, 4]	0·1824	0·1810	0·1685	0·1678
[3, 2]	0·1833	0·1837	0·1692	0·1684
[2, 3]	0·1899	0·1819	0·1674	0·1681

	$q = 7$ ($v_0 = 0{\cdot}1545$)	$q = 8$ ($v_0 = 0{\cdot}1449$)
	χ	χ
[5, 2]	0·1602*	0·1505*
[4, 3]	0·1579	0·1488
[3, 4]	0·1567	0·1476
[4, 2]	0·1585	0·1497
[3, 3]	0·1587	0·1504
[3, 2]	0·1578	0·1485

interpret these results as evidence supporting the conjecture that the singularities of both the χ and χ_3 series are both exactly at v_0, even when the system undergoes a first-order transition. It then follows that the power law divergence of any thermodynamic quantities at v_0 by itself cannot be used as a criterion for the existence of a continuous transition, and that the metastable state which the MFA predicts cannot exist, at least through v_0.

4. Analysis of series in three dimensions

In this section we utilize high-temperature series of the type given by equation (13) to investigate the nature of the phase transition in three dimensions. The method we have adopted in our work is to look directly at the phase space. For this purpose we consider a subspace of the field space, $\zeta_1 \geqslant 0$ and $\zeta_i = 0\,(i \geqslant 2)$, and for simplicity consider $q = 3$. For higher q the following arguments are easily generalized.

Straley and Fisher (1973) have sketched out the field space phase diagram for both the case of a continuous and of a discontinuous transition in zero field (see their figures 2 and 9). In the former case, for $\tau > 0$, $\zeta_2 = \zeta_3 = 0$, there are no singularities in the free energy $f(\tau, v)$ for any v, so that a high-temperature expansion of the form given by equation (13) will be valid up to the $\tau = 0^+$ contour, which forms the phase boundary for $m \geqslant 0$. For the discontinuous case $\tau = 0^+$ forms only a part of the phase boundary (ie for $v > v_0$ in figure 1). The cross section of the first-order coexistence surface (w_1 of

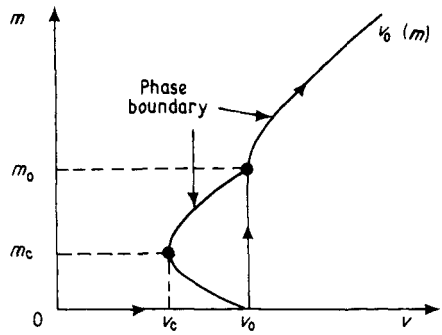

Figure 1. Schematic of relation of phase boundary to zero-field magnetization $v_0(m)$ for the case of a first-order transition in the Potts model. The point (m_c, v_c) is a critical point and m_0 is the zero-field magnetization jump at the transition temperature v_0.

Straley and Fisher 1973) with the $\zeta_2 = \zeta_3 = 0$ plane in the field space will, in the m–v plane, give the rest of the phase boundary as shown in figure 1. In particular, at the point (m_c, v_c) the 'susceptibility' $\partial^2(-\beta f)/\partial\zeta_1^2$ diverges strongly in the sense of Griffiths and Wheeler (1970), since the ζ_1 (ie τ) direction is the strong direction on the corresponding point in the field space. Therefore, if we consider the series

$$\frac{\mathrm{d}\tau}{\mathrm{d}m} = \sum_{n=0}^{\infty} C_n(m) v^n \tag{20}$$

for which only a finite number of terms are known, and if we approximate the solution to the equation $\mathrm{d}\tau/\mathrm{d}m = 0$ for fixed m by constructing appropriate PA to the series, we should then reasonably expect to see the effect of the critical point (m_c, v_c) for some finite m_c if there is a first-order transition.

Since there is some controversy as to whether the 'spinodal curve' on which the analytic continuation of $d\tau/dm$ vanishes really exists (Gaunt and Baker 1970 and references therein), $d\tau/dm$ might vanish only at the true critical point. However, any finite length series will obviously tend to give a more-or-less definite spinodal curve around the critical point. Accordingly, we denote by $v_{sp}(m)$ this 'effective' spinodal curve which is estimated by the PA.

Furthermore, we can approximate the $\tau(v, m) = 0$ locus, which we denote by $v_0(m)$, from the smallest positive real pole with positive residue of the PA to the logarithmic derivative of the τ series for fixed m. This method of determining the phase boundary was first successfully applied to the Ising and Heisenberg models by Baker *et al* (1970) and Gaunt and Baker (1970). Then for a continuous transition we should expect to obtain a monotonically increasing $v_0(m)$ as m increases from zero if the series is long enough, while for a discontinuous transition, for $m < m_0$ where $\tau(v, m) = 0$ is a straight line and within the two-phase region, we should obtain a curve which is basically the analytic continuation of $v_0(m)$ for $m > m_0$ since the zeros of the PA themselves are analytic functions of m as long as we handle finite length series. In any case, as $m \to 0^+$, the $d\tau/dm$ and τ/m series become identical ($= \chi^{-1}$) and $v_0(m = 0)$ is the point where the zero-field susceptibility diverges. For a first-order transition, $v_0(0)$ may not necessarily be the transition temperature (as in the MFA). However, the numerical evidence discussed in § 3 for the two-dimensional case suggests the possibility that $v_0(0) = v_0$.

We have concentrated most of our attention on the FCC lattice in the belief that FCC series are more rapidly converging than for the other cubic lattices, for a given length. First we consider the $q = 3$ FCC lattice. The general trend of the $v_0(m)$ and $v_{sp}(m)$ curves, obtained by constructing PA to $D \lg \tau$ and $D \lg(d\tau/dm)$ respectively for a given value of m, is that as m increases from zero they decrease from the $m = 0$ value, reaching a minimum in v around $m \sim \frac{1}{3}$ and $m \sim 0{\cdot}2$ for τ/m and $d\tau/dm$ respectively, and then start to increase again. There is extremely good convergence between different PA around their respective minimum. In figure 2 we sketch this 'trend' of the poles by taking the average of the values for the [3, 2], [4, 2], [3, 3], [5, 2], [4, 3] and [3, 4] PA.

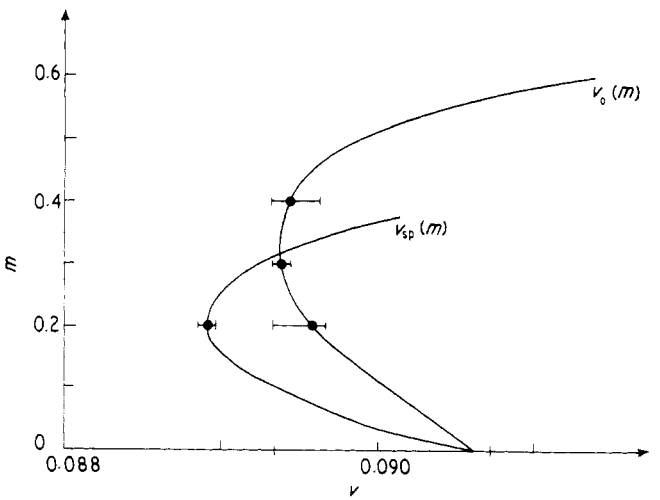

Figure 2. Plot of $v_0(m)$ and $v_{sp}(m)$ for $q = 3$ on the FCC lattice. The error bars, shown for a few selected points, are determined from a ratio test of the inverse of the appropriate series.

A few anomalous poles which have an interfering real pole-zero pair in their neighbourhood are omitted when taking the average. This figure shows striking similarity with the MFA for a first-order transition. Now the question is whether these 'bumps' are really due to a first-order transition or whether they are just spurious numerical effects near the tricritical point due to the shortness of our series. If they are indeed due to a first-order transition, we would expect that the minimum of $v_{sp}(m)$ ($v \sim 0{\cdot}0889$ at $m \sim 0{\cdot}21$) which supposedly corresponds to the critical point (m_c, v_c) in figure 1, must clearly be lower than $v_{sp}(0)$. Unfortunately, the Padé entries for $m = 0$ have too many anomalies to enable us to reliably estimate $v_{sp}(0)$.

Our analysis of the χ_3 series for the two-dimensional lattices, however, suggests not only that the location of the singularity of χ_3 is the same as that of χ but also that frequently the PA of $D \lg \chi_3$ give a better estimate for the known transition temperature than χ (see for example $q = 5$ for the SQ lattice). This motivated us to consider the χ_3 series together with χ. Table 3 shows the poles and residues of the PA to $D \lg \chi_3$ together with those for χ. It is apparent that the results shown in this table enable us to make a more confident estimate of the location of the singularity than that of χ alone. Also shown in table 3 are the poles and residues of the PA to $D \lg(d\tau/dm)$ at $m = 0{\cdot}21$. From this table one would conclude that $dm/d\tau\,(m = 0{\cdot}21)$ diverges at $v \sim (889 \pm 2) \times 10^{-4}$ with an exponent 1·15 while χ_3, and hence also χ, diverges at $v \sim (905 \pm 10) \times 10^{-4}$. These estimates have to be interpreted within the limitations that the series are not long enough to show convergence in the sequences for the $[N, N \pm j]$ approximants. For example, the sequence of poles (multiplied by 10^5) of the $[N, N-1]$ approximants are for $N = 1, 2, 3$ and 4, 12500, 9235, 9004 and 9036 respectively, for χ_3 and 8063, 9603, 8879 and 8893 respectively, for $dm/d\tau\,(m = 0{\cdot}21)$. The difference between the estimated $v_{sp}(0{\cdot}21)$ and $v_0(0)$ is not large enough to conclude absolutely that $v_{sp}(0{\cdot}21) < v_0(0)$. However, we feel that this is indeed the case in view of the excellent convergence between different approximants and hence favour the transition being of first order. Assuming that the transition is of first order, the bump in $v_0(m)$ can be understood as resulting from the analyticity of the poles as a function of m, since by enforcing the analyticity

Table 3. Physical poles (multiplied by 10^5) and residues of PA to the logarithmic derivative of χ^{-1}, χ_3^{-1} and $d\tau/dm\,(m = 0{\cdot}21)$ series for $q = 3$ for the FCC lattice. *: see table 2 for explanation; a, b, c: these approximants have a smaller real pole at 8311, 7722, 8585, with a residue 0·10, 0·07, 0·26 for a, b, c respectively, immediately followed by a real zero. These pole-zero pairs are not close enough to each other to ignore completely as for the other starred entries. However, they have too small a residue to be considered as physical. Hence we disregard these three entries from further consideration.

PA	χ^{-1} Pole	Residue	χ_3^{-1} Pole	Residue	$d\tau/dm\,(m = 0{\cdot}21)$ Pole	Residue
[5, 2]	9154*	0·95*	9043	2·41	8891	1·15
[4, 3]	9057	0·98	9036	2·39	8893	1·15
[3, 4]	9212*	0·89*[a]	9175*	2·45*[b]	8892	1·15
[2, 5]	9329*	0·74*[c]	9023	2·37	8892	1·15
[4, 2]	9018	0·95	9061	2·44	8888	1·14
[3, 3]	9016	0·95	9054	2·43	8891	1·15
[2, 4]	9068*	0·99*	9064	2·45	8898	1·15
[3, 2]	9037	0·97	9004	2·33	8879	1·14
[2, 3]	9052	0·98	9078	2·47	8903	1·15

the straight line portion of the $\tau = 0$ curve will turn out to be more or less mean-field-like as long as we have finite length series.

For $q = 4$ and 5 on the FCC we have results qualitatively similar to that in the $q = 3$ case. The minimum of $v_{sp}(m)$ [$v_0(m)$] occurred approximately at $m \sim 0{\cdot}3$[0·5] and 0·35[0·6] for $q = 4$ and 5 respectively, and the poles of the PA to the $D \lg \chi$ and $D \lg \chi_3$ which are to be compared with those of $dm/d\tau$ at $m = 0{\cdot}3$[0·35] for $q = 4$[5] are listed in table 4 for the six most significant PA. From this we might take $v_0 = (815 \pm 10) \times 10^{-4}$ and $v_{sp}(0{\cdot}3) = (776 \pm 10) \times 10^{-4}$ for $q = 4$ and $v_0 = (755 \pm 10) \times 10^{-4}$ and $v_{sp}(0{\cdot}35) = (682 \pm 10) \times 10^{-4}$ for $q = 5$. Hence we have a much better situation here than for the $q = 3$ case and we can more clearly see that v_0 is higher than the spinodal point. Since the MFA is supposedly more meaningful for higher dimensions and higher q (Mittag and Stephen 1974) and since $q = 4$ is the dividing point between the second- and first-order transitions in two dimensions, one would expect that the dividing point in three dimensions should be between 2 and 4 and the above analysis suggests that the transition is of first order, at least for $q \geqslant 3$.

Table 4. Physical poles (multiplied by 10^5) of PA to $D \lg \chi$, $D \lg \chi_3$ and $d\tau/dm$ at $m = 0{\cdot}3$ (0·35) for $q = 4$ (5) for the FCC lattice. The residues of the poles for χ^{-1} are given in parentheses.

	$q = 4$ FCC			
PA	χ		χ_3	$d\tau/dm$ ($m = 0{\cdot}3$)
[5, 2]	8175	(0·75)	8130	7759
[4, 3]	8171	(0·74)	8113	7759
[3, 4]	8173	(0·75)	8115	7757
[4, 2]	8194	(0·77)	8191	7757
[3, 3]	8187	(0·76)	8145	7768
[3, 2]	8230	(0·79)	8259	7715
	$q = 5$ FCC			
PA	χ		χ_3	$d\tau/dm$ ($m = 0{\cdot}35$)
[5, 2]	7564	(0·64)	7536	6819
[4, 3]	7563	(0·64)	7536	6820
[3, 4]	7563	(0·64)	7543	6803
[4, 2]	7572	(0·64)	7542	6828
[3, 3]	7565	(0·64)	7425	6857
[3, 2]	7613	(0·67)	7642	6738

The SC and BCC series were also investigated in the same way, for $q = 3$ and 4. Although the convergence between different PA was appreciably degraded compared to the FCC case, all the general features of the FCC lattice were found. In particular, the values of m where the minimum of $v_{sp}(m)$ and $v_0(m)$ occurred were approximately the same as for the FCC lattice for both lattices for given q. The locations of $v_{sp}(0) = v_0$ and $v_{sp}(m_c)$ were estimated to be:

$v_0 = (200 \pm 2) \times 10^{-3}$, $v_{sp}(0{\cdot}2) = (196 \pm 2) \times 10^{-3}$ for $q = 3$ SC

$v_0 = (1415 \pm 10) \times 10^{-4}$, $v_{sp}(0{\cdot}2) = (139 \pm 1) \times 10^{-3}$ for $q = 3$ BCC

$v_0 = (186 \pm 3) \times 10^{-3}$, $v_{sp}(0{\cdot}3) = (176 \pm 5) \times 10^{-3}$ for $q = 4$ SC

$v_0 = (1305 \pm 15) \times 10^{-4}$, $v_{sp}(0{\cdot}3) = (123 \pm 5) \times 10^{-3}$ for $q = 4$ BCC;

hence $v_0 > v_{sp}(m_c)$ for all cases. A similar analysis was attempted for both the plane square and plane triangular lattices where the answer is known. Unfortunately, due to severe numerical uncertainties, no conclusion as to the relative positions of v_0 and $v_{sp}(m_c)$ could be drawn.

From the residues for the χ series listed in tables 3 and 4 and from the evidence shown for the two-dimensional lattices (§ 3), the asymptotic behaviour of χ near the transition may be described as

$$\chi \sim (v_0 - v)^{-\gamma(q)} \tag{21}$$

with

$$\begin{aligned} \gamma(3) &= 0{\cdot}95 \pm 0{\cdot}1 \\ \gamma(4) &= 0{\cdot}75 \pm 0{\cdot}1 \\ \gamma(5) &= 0{\cdot}64 \pm 0{\cdot}1. \end{aligned} \tag{22}$$

Also, from table 3 we can estimate γ_3 for $q = 3$ to be $2{\cdot}4 \pm 0{\cdot}1$. These exponents estimated from an eight-term series for the FCC lattice are to be compared with the results $\gamma(3) = 0{\cdot}9 \pm 0{\cdot}1$ and $\gamma_3(3) = 2{\cdot}1 \pm 0{\cdot}2$ estimated by Straley (1974) from his nine-term series for the SC lattice.

5. Discussion

For $q = 3$ and in two dimensions, the tricritical point discussed here is not the kind usually studied. Hence it poses an interesting problem for study by means of the scaling hypothesis. In fact Straley (1974) has proposed a form for the singular part of the free energy which predicts that $\alpha = \alpha' = 2 + 3\gamma - 2\gamma_3$ and that $\gamma = \gamma'_\perp$ (for the definition of $\gamma'_\perp$ see Straley and Fisher 1973). It was found by these authors that $\gamma' = 1{\cdot}5 \pm 0{\cdot}2$, $\gamma'_\perp = 1{\cdot}1 \pm 0{\cdot}1$, $\alpha = \alpha' = 0{\cdot}05 \pm 0{\cdot}10$ and $\beta = 0{\cdot}10 \pm 0{\cdot}01$. On the other hand Zwanzig and Ramshaw (1973 preprint), on re-analysing the free energy series of Kihara *et al* (1954) by a new method, estimated that $\alpha = \alpha' = 0{\cdot}286 \pm 0{\cdot}02$. Using the values $\gamma = 1{\cdot}42$ and $\gamma_3 = 3{\cdot}00$ found in § 3 and the first relation of Straley, given above, we see that $\alpha = \alpha' = 0{\cdot}26$ which is in agreement with the latter work. Furthermore it does not contradict the strict thermodynamic inequality $\alpha' + 2\beta + \gamma' \geqslant 2$ which Straley and Fisher, using their value of α, found difficulty in satisfying. Moreover, $\gamma = \gamma'_\perp$ cannot be accepted as true, based on the available data. Hence we feel that more investigation regarding this point is necessary.

Evidence presented above for the divergence of both χ and χ_3 at the first-order transition point suggests that it is possible that other thermodynamic quantities might behave in a similar manner to those near a critical point except for finite discontinuities in the first derivatives of the free energy; for example, $m \sim m_0 + A|T - T_0|^\beta$ ($m_0 > 0$). This sort of situation is in fact actually observed in liquid crystals. Stinson and Litster (1970) observed a divergence of the magnetic birefringence and a divergence and critical slowing down of the fluctuations in the order parameter as the temperature is lowered to the first-order isotropic-to-nematic transition, while the metastable states could not be observed. Their data showed that the inverse of the fluctuation in the order, ie the

inverse susceptibility in our language, while obeying the MFA prediction $\chi^{-1} = A(T - T_c^*)$ (T_c^* being ~ 1 K higher than T_0, the transition temperature) accurately for temperatures several degrees higher than T_0, definitely deviates in a downward direction from the linear behaviour near T_0, suggesting the possibility of the vanishing of χ^{-1} at T_0, ie $\chi^{-1} \sim (T - T_0)^\gamma$ as $T \to T_0^+$ with $\gamma < 1$. This is in contrast to the usual para- to ferromagnetic transition where χ^{-1} deviates from a linear behaviour so as to give $\gamma > 1$. It would be desirable to have more experimental data in the transition region, but if this is indeed the case the Potts model seems to predict these pre-transitional phenomena correctly for some appropriate value of q.

Acknowledgments

We wish to thank Professor M E Fisher for helpful comments.

Appendix

A.1. Coefficients of $\chi = q^{-1}(1 + \Sigma_{n=1}^{\infty} a_n v^n)$ *series for* SQ *and* TR *lattices*

The numbers in parentheses are the values of q.

	SQ(3)	SQ(4)	SQ(5)	SQ(6)	TR(3)
a_1	4	4	4	4	6
a_2	12	12	12	12	30
a_3	36	36	36	36	150
a_4	112	124	136	148	726
a_5	316	356	396	436	3456
a_6	952	1164	1376	1588	16254
a_7	2672	3492	4432	5492	75876
a_8	7812	10748	13980	17508	351852

	TR(4)	TR(5)	TR(6)	TR(7)	TR(8)
a_1	6	6	6	6	6
a_2	30	30	30	30	30
a_3	162	174	186	198	210
a_4	846	966	1086	1206	1326
a_5	4398	5412	6498	7656	8886
a_6	22662	30042	38394	47718	58014
a_7	116430	166956	228174	300804	385566
a_8	596730	928056	1357710	1897572	2559522

A.2. Coefficients of $\chi_3 = q^{-2}(q-2)(1 + \Sigma_{n=1}^{\infty} b_n v^n)$ *series for the* SQ *and* TR *lattices*

The numbers in parentheses are the value of q.

	SQ(3)	SQ(4)	SQ(5)	SQ(6)
b_1	12	12	12	12
b_2	72	72	72	72
b_3	348	348	348	348
b_4	1452	1512	1572	1632

	SQ(3)	SQ(4)	SQ(5)	SQ(6)
b_5	5652	6060	6468	6876
b_6	20772	23472	26172	28872
b_7	73560	87036	101352	116508
b_8	252588	316488	385284	458976

	TR(3)	TR(4)	TR(5)	TR(6)
b_1	18	18	18	18
b_2	180	180	180	180
b_3	1398	1446	1494	1542
b_4	9540	10404	11268	12132
b_5	60120	69930	80100	90630
b_6	358728	448668	546756	652992
b_7	2056608	2783538	3625128	4585698
b_8	11434878	16830612	23512806	31594860

A.3. Polynomials $\psi_n(m)$ for $q = 3$ on the face-centred cubic lattice

(See equation (14))

$$\psi_0 = 1$$

$$\psi_1 = -12-12m+24m^2$$

$$\psi_2 = 12+102m-246m^2-492m^3+624m^4$$

$$\psi_3 = -12-60m+1128m^2+5736m^3-5784m^4-16944m^5+15936m^6$$

$$\psi_4 = 24+870m-4338m^2-29817m^3+27531m^4+256746m^5-113400m^6-544464m^7 + 406848m^8$$

$$\psi_5 = -156+4164m-1584m^2+80256m^3-98916m^4-1906188m^5-199656m^6 + 9711360m^7-1198176m^8-16790592m^9+10399488m^{10}$$

$$\psi_6 = -1080+38490m-91590m^2-191568m^3+564852m^4+8839890m^5+5747394m^6 - 87885756m^7-54497352m^8+330801456m^9+33351360m^{10} - 502440960m^{11}+265764864m^{12}$$

$$\psi_7 = -13176+316476m-624636m^2+784944m^3-549072m^4-32620836m^5 - 30137292m^6+532745208m^7+787809984m^8-3367464816m^9 - 3474596928m^{10}+10506629568m^{11}+2998609920m^{12} - 14711920128m^{13}+6791030784m^{14}$$

$$\psi_8 = -149958+2826756m-6009762m^2+3535149m^3+5629503m^4+78228720m^5 + 114601260m^6-2487973371m^7-5552550453m^8+22931115888m^9 + 52070929212m^{10}-111741997584m^{11}-165637920240m^{12} + 315776346336m^{13}+144803133312m^{14}-423918550272m^{15} + 173558805504m^{16}.$$

References

Alexander S and Yuval G 1974 *J. Phys.* C: *Solid St. Phys.* **7** 1609–20
Amit D J and Shcherbakov A 1974 *J. Phys.* C: *Solid St. Phys.* **7** L96–8
Baker Jr G A, Eve J and Rushbrooke G S 1970 *Phys. Rev.* B **2** 706–21
Baker Jr G A, Gilbert H E, Eve J and Rushbrooke G S 1967 *Brookhaven National Laboratory Rep.* No. 50053 (T-460)
Baxter R J 1973 *J. Phys.* C: *Solid St. Phys.* **6** L445–8
Chang T S, Hankey A and Stanley H E 1973 *Phys. Rev.* B **8** 346–64
Ditzian R V and Oitmaa J 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** L61–4
Domb C 1960 *Adv. Phys.* **9** 149–361
Enting I G 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** 1617
Gaunt D S and Baker Jr G A 1970 *Phys. Rev.* B **1** 1184–210
Golner G R 1973 *Phys. Rev.* B **8** 3419–22
Griffiths R B and Wheeler J C 1970 *Phys. Rev.* A **2** 1047–64
Kihara L, Midzuno Y and Shizume T 1954 *J. Phys. Soc. Japan* **9** 681–7
Kim D and Joseph R I 1974a *J. Phys.* C: *Solid St. Phys.* **7** L167–9
—— 1974b *Phys. Lett.* A **46** 359–60
Mittag L and Stephen M J 1971 *J. Math. Phys.* **12** 441–50
—— 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** L109–12
Potts R B 1952 *Proc. Camb. Phil. Soc.* **48** 106–9
Priest R G 1971 *Phys. Rev. Lett.* **26** 423–5
Stinson III T W and Litster J D 1970 *Phys. Rev. Lett.* **25** 503–6
Straley J P 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** 2173–80
Straley J P and Fisher M E 1973 *J. Phys.* A: *Math., Nucl. Gen.* **6** 1310–26