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Three-dimensional Potts model

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Abstract. The thermodynamic functions for the three-component Potts model on a simple cubic lattice are constructed as a low-temperature, high-field series and also as a high-temperature, low-field series. Both series predict divergences in the relevant compliances in the same temperature range, which may be evidence for a continuous phase transition. The critical exponents are tentatively determined, and related to a proposed theory for the Potts tricritical point.

1. Introduction

The Potts model is a generalization of the standard Ising model in which each site of a lattice can be in one of q distinct states (Potts 1952, Mittag and Stephen 1971). Nearest neighbour sites interact with an energy ϵ_0 if they are in the same state, and an energy ϵ_1 if they differ. There may also be external fields $\zeta_1, \zeta_2, \ldots, \zeta_q$ which favour a site being in one or another of the states. In what follows we will take $\epsilon_0 = 1, \epsilon_1 = 0$, and present some numerical studies of the $q = 3$ Potts model on the simple cubic lattice.

Previous work (Straley and Fisher 1973, to be referred to as SF; Baxter 1973) has indicated that the two-dimensional Potts model has a continuous ('second-order') phase transition and exhibits an unusual type of tricritical point; in contrast, Landau theory indicates a first-order transition should occur (SF). Since this theory presumably is correct for large dimensionality, it is certainly of interest to see whether the physically relevant case of three dimensions exhibits the tricritical phenomenon. The model is harder to analyse in three dimensions than in two because there is no dual symmetry (see Mittag and Stephen 1971): we do not know where the phase transition takes place. It is not sufficient, of course, to establish the existence of a divergence of some compliance as a 'critical temperature' is approached from one side; this could equally well be the locus of a continuous transition or the limit of stability of a phase superheated beyond a first-order transition. It is necessary to study the state functions both above and below the putative critical point, and establish that the series for the compliance predict divergences at the same temperature, which must also be the temperature where the free energies of the ordered and disordered phases become equal.

There are several previous discussions of the present problem in the literature. (i) Golner (1973) has used the Wilson (1971) recursion integral equations in a study of an analogous model—essentially an XY model with a cubic-order perturbation. He finds evidence for a first-order transition for a certain arbitrarily chosen strength of this perturbation. Amit and Shcherbakov (1974) have shown that in an ϵ expansion the transition is first order for all values of the perturbation. It may be, however, that these models, which replace the lattice of sites that are in three distinct states by a continuously varying two-dimensional field, fail to be faithful representations of the three-dimensional Potts model (their conclusions evidently do not apply in two dimensions). (ii) Ditzian and Oitmaa (1974) have recently constructed the high-temperature series for the Ising $S = 1$ model with a biquadratic interaction, which becomes the Potts $q = 3$ model for a certain value of the biquadratic parameter. They find that the Potts model case lies slightly outside the range of parameter which allows a continuous transition. This conclusion, that the Potts model has a first-order transition but with small discontinuities at the transition, is a possible alternative interpretation to the studies to be presented below.

The interpretation which will be preferred, however, is that a continuous transition occurs near

$$\exp\left(-\frac{1}{T_t}\right) = 0{\cdot}585 \qquad (T_t = 1{\cdot}87),$$

with exponents as given in table 1.

Table 1. Critical exponents.

Function	Exponent	Value	
C	α'	$-0{\cdot}05 \pm 0{\cdot}1$	$T < T_t$
M	β	$0{\cdot}25 \pm 0{\cdot}05$	
χ	γ'	$1{\cdot}3 \pm 0{\cdot}1$	
χ_3	γ'_3	$2{\cdot}7 \pm 0{\cdot}2$	
$\chi_\perp$	$\gamma'_\perp$	$0{\cdot}8 \pm 0{\cdot}1$	
χ	γ	$0{\cdot}9 \pm 0{\cdot}1$	$T > T_t$
χ_3	γ_3	$2{\cdot}1 \pm 0{\cdot}2$	

2. Low-temperature expansion

The low-temperature expansion was performed as discussed in SF. In the limit of lowest temperatures, all sites will be in the same state (say 3); the leading terms in the partition function will be those for which only a small density of sites are in other states (1 and 2). The expansion parameters are

$$x = \exp(-1/T) \tag{1}$$

and

$$y_1 = \exp(\zeta_1/T), \qquad y_2 = \exp(\zeta_2/T). \tag{2}$$

With the aid of the tables of lattice constants given by Domb (1960), this expansion of the free energy was carried through terms in x^{24}, which includes all terms through fourth order in the variables y_1 and y_2. The series may also be characterized as containing all contributions from clusters in which four sites are in minority states. The series is given in appendix 1. This series was used to construct series for the temperature derivative of the specific heat, the order parameter, the two susceptibilities, and one further quantity

$$\chi_3 = -T^2\left(\frac{\partial}{\partial\zeta_1}+\frac{\partial}{\partial\zeta_2}\right)^3 F(T,\zeta_1,\zeta_2), \tag{3}$$

all evaluated at zero field. These series are listed in table 2.

Table 2. Low-temperature series.

	F	M	χ	$\chi_\perp$	χ_3
x^0	0	1	0	0	0
x^6	2	-3	2	2	2
x^{10}	6	-18	24	24	48
x^{11}	6	-18	24	0	48
x^{12}	-14	42	-56	-28	-112
x^{14}	30	-135	270	270	810
x^{15}	60	-270	540	60	1620
x^{16}	-108	477	-930	-594	-2694
x^{17}	-144	648	-1296	-144	-3888
x^{18}	$372\frac{2}{3}$	-1980	4768	3264	17536
x^{19}	498	-2988	7968	1488	31872
x^{20}	-714	4140	-10560	-9048	-39840
x^{21}	-2366	14052	-36992	-5600	-145568
x^{22}	3270	-21690	64812	41892	294540
x^{23}	7704	-52920	163440	31008	765360
x^{24}	-8126	55200	-166184	-127912	-744536
	$\sim\Delta^{2-\alpha'}$	$\sim\Delta^{\beta}$	$\sim\Delta^{-\gamma'}$	$\sim\Delta^{-\gamma'_\perp}$	$\sim\Delta^{-\gamma'_3}$

$\Delta = T_c - T$.

3. High-temperature expansions

Mittag and Stephen (1971) have discussed a method for generating high-temperature expansions in the absence of external fields. Their method may be generalized to allow for the presence of such fields, with the result that the partition function may be written as

$$Z = \left(\frac{1+2x}{3}\right)^{3N}\left(\frac{y_1+y_2+y_3}{3}\right)^N \operatorname{Tr}\prod_{nn}[I+v(\Omega_r\Omega_s^\dagger+\Omega_r^\dagger\Omega_s)]\prod_s(I+\eta^*\Omega_s+\eta\Omega_s^\dagger) \tag{4}$$

where $v = (1-x)/(1+2x)$ is the high-temperature expansion variable,

$$\eta = \frac{y_1+y_2\omega+y_3\omega^2}{y_1+y_2+y_3}, \qquad \omega = -\tfrac{1}{2}+\tfrac{1}{2}\sqrt{3}\mathrm{i} \tag{5}$$

and Ω_r is a 3×3 matrix attached to site r which has the properties that $\Omega_r^\dagger\Omega_r = \Omega_r^3 = I$ (the unit matrix) so that $\operatorname{Tr}(\Omega^p\Omega^{\dagger q}) = 3$ if $p-q$ is a multiple of 3, and vanishes otherwise. The first product contains all pairs of sites r and s that are nearest neighbours; the second runs over all sites in the lattice.

The non-vanishing terms in the product can be represented as directed weak graphs, in which each factor of $v\Omega_r\Omega_s^\dagger$ becomes a bond directed from s to r. Unlike some other directed-graph systems, the number of bonds coming out of a vertex does not strictly have to balance the number coming in: the property $\Omega_r^3 = I$ allows three incoming bonds to 'annihilate', thus breaking the 'current conservation'. The terms $\eta\Omega_s^\dagger$ from the second product become root points which emit a line (or absorb two). Some typical graphs are illustrated in figure 1.

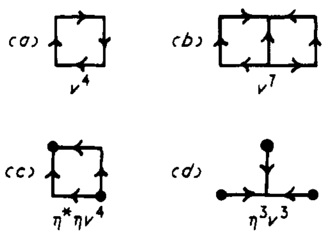

Figure 1. Typical graphs entering into the high-temperature series. (*a*) A contribution to the zero-field free energy (and specific heat). (*b*) Another such graph, which exhibits vertices of odd order. (*c*) A contribution to the susceptibility χ. (*d*) A contribution to the susceptibility χ_3.

The free energy function thus calculated may be grouped into terms

$$-F/kT = \mathscr{F}_{\text{reg}} + \mathscr{F}_1(v) + \eta\eta^*\mathscr{F}_2(v) + (\eta^3 + \eta^{+3})\mathscr{F}_3(v) + \dots \tag{6}$$

where

$$\mathscr{F}_{\text{reg}} = 3\ln(1+2x) - 3\ln 3 + \ln(y_1 + y_2 + y_3), \tag{7}$$

and $\mathscr{F}_1, \mathscr{F}_2, \mathscr{F}_3 \dots$ have series expansions in v, which are given in table 3. The lattice constants were taken from the tables of Baker *et al* (1967); construction of the series thus reduced to selecting the relevant graphs, determining the possible assignments of root points, and establishing the number of ways each group can be directed consistent with the vertex rules. Two susceptibilities of the model were considered: $\chi = 1 + \mathscr{F}_2(v)$, and $\chi_3 = \frac{1}{3} + \mathscr{F}_3(v)$. The former series is just the usual susceptibility $-\frac{1}{2}T(\partial^2 F/\partial\zeta_1^2)$ and is independent of the 'direction of ζ' (that is, it depends only on $\zeta_1^2 + \zeta_2^2 + \zeta_3^2 - \frac{1}{3}(\zeta_1 + \zeta_2 + \zeta_3)^2$).

Table 3. High-temperature series.

	$\mathscr{F}_1$	$\mathscr{F}_2$	$\mathscr{F}_3$
v^1	0	6	0
v^2	0	30	15
v^3	0	150	170
v^4	6	762	1389
v^5	0	3774	10068
v^6	44	19170	67123
v^7	36	95298	428250
v^8	402	482190	2631723
v^9	688	2375322	15800472
v^{10}	1596		

The latter series is related to the third field derivatives of F and does depend on the direction of ζ; it was introduced originally in response to the idea that the relevant compliance ought to depend on the sign of ζ_1 (ie the direction of ζ). We will see below that χ and χ_3 contain essentially the same information about the tricritical exponents.

4. Series analysis

Whatever the order of the transition, its position is defined by the condition that the free energies of ordered and disordered phases become equal at the transition temperature. The transition will be called continuous if the temperature derivative of the free energy is continuous at this temperature. Since both high- and low-temperature series for the free energy have been derived, we should try to use this definition. The question was approached by assuming that the series $(x\,\partial/\partial x)^3F(x)$ and $(v\,\partial/\partial v)^3F_{\text{sing}}(v)$ (which both are the product of regular functions and the temperature derivative of the specific heat) have a singularity of index -1, approximately. Padé approximants to these series were found which exhibited simple poles at $x = 0{\cdot}5856$ (for [15, 9]) and $v = 0{\cdot}1977$ (for [7, 3]), respectively (which correspond to similar temperatures). These approximants were integrated numerically to construct $F(x)$ and $F_{\text{sing}}(v)$. The results are shown in figure 2. The free energies of the two phases are nearly the same in the interval $1{\cdot}8 < T < 1{\cdot}9$, and the internal energies are the same for $T = 1{\cdot}88$.

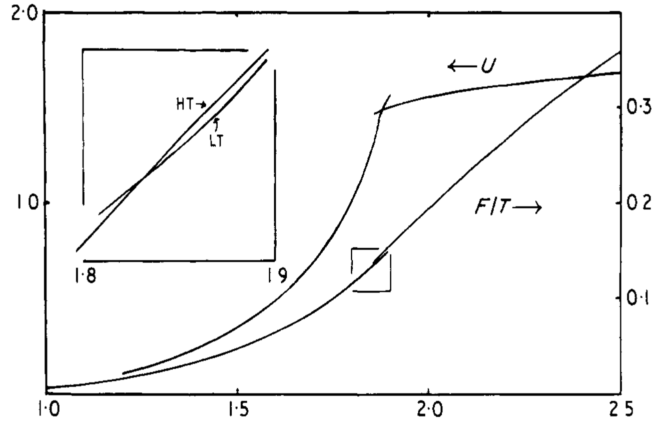

Figure 2. The free energy and internal energy near the tricritical point. The high- and low-temperature series have been used to construct approximations to U and F. The high-temperature (HT) and low-temperature (LT) approximations to F agree in the interval $1{\cdot}8 < T < 1{\cdot}9$ (inset), and the two approximations for U take on the same value near $T = 1{\cdot}88$.

This construction can only be regarded as a consistency check: the assumption that the free energy has singular derivatives at a unique temperature virtually contains the assumption that the transition is continuous; and the contrary assumption that the free energy is regular would surely have led to the conclusion that the transition is first order. (This criticism is also relevant to the similar construction performed in SF. In its defence, we will point out that the Padé approximants to the low-temperature series for $(x\,\partial/\partial x)^3F$ nearly all give simple poles near the indicated T_t, and that its success is not guaranteed by the assumption introduced—whereas showing a discontinuity in U is consistent with regular F is trivial). In any case, the high-temperature series was too short to be reliable, and finagling with the approximations to $\partial c/\partial T$ will change the agreement for better or worse.

The conjecture that there is a continuous phase transition near $T_t = 1{\cdot}87$ implies that all compliances should also be divergent there. This possibility was studied by constructing Padé approximants to the logarithmic derivatives of the relevant series, as was done in SF. The results are shown in figure 3, in which the residues at the pole of the approximants (= predicted critical exponents) are plotted against the position of the pole. The latter have been translated into the temperature scale in order to allow direct comparison of the high- and low-temperature series results.

The low-temperature series have more terms (but not more information). The Padé analysis of the low-temperature series thus gives more guesses (corresponding to the larger number of possible partitions $L = M \leqslant N$) and can be interpreted more reliably. It should be mentioned that many of the approximants to the low-temperature χ_3 predicted no transition or predicted a transition well off figure 3; the series for low-temperature $\partial c/\partial T$ and M suffered mildly from the same disease. The high-temperature series are regular enough that ratio test analysis is possible; the corresponding predictions have also been entered in figure 3.

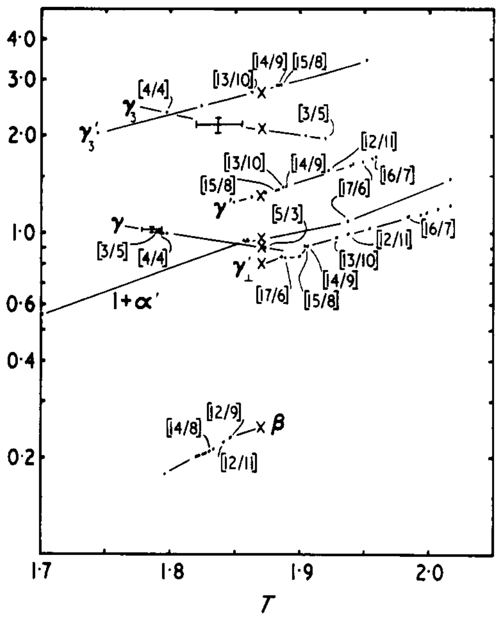

Figure 3. Predicted exponents and tricritical temperatures. Padé approximants have been constructed to the logarithmic derivative of each series of interest; here are plotted pole residue against pole position, which may be interpreted as predicted T_t. The symbol (⊢⫨⊣) represents the results of a ratio analysis of the high-temperature series. The symbol (×) represents the values chosen for table 1.

5. Relationship to scaling theory

Inspection of table 1 reveals an unusual feature: the exponents above the transition are different from those below. A similar anomaly is present in the studies of the two-dimensional Potts model, where $\gamma' = 1\cdot5$–$1\cdot7$ (according to the analysis of SF; the Rushbrooke inequality forces the upper value to be taken), and $\gamma = 1\cdot4 \pm 0\cdot1$ (Kim and Joseph 1974, Straley, unpublished). These relationships are anomalous in that they are contrary to experience with the Ising model and other systems; as we shall see below, they are also in conflict with the predictions of the Griffiths (1973) scaling theory.

The geometry of the Potts tricritical point was discussed in SF. The symmetry of the model requires that it be the intersection of a line of first-order transitions (at $\zeta_1 = \zeta_2 = \zeta_3$, for $T < T_t$) and three critical lines which lie symmetrically in the $(\zeta_1, \zeta_2, \zeta_3)$ space above T_t (see figure 2 of SF). If we define the variables t, ζ_0, ζ, and θ by

$$t = T - T_t, \qquad \zeta_1 + \zeta_2 + \zeta_3 = 3\zeta_0,$$
$$\zeta_1 = \zeta_0 + \zeta\cos\theta, \qquad \zeta_2 = \zeta_0 + \zeta\cos(\theta + \tfrac{2}{3}\pi), \tag{8}$$

then the Griffiths theory, adapted to the present geometry, becomes the assumption that the singular part of the free energy has the scaling behaviour

$$F_{\text{sing}}(t, \zeta, \zeta^2 \sin^2 \tfrac{3}{2}\theta) = \lambda^{-2+\alpha_t} F_{\text{sing}}(\lambda^{\phi_t} t, \lambda\zeta, \lambda^{2\Delta_t}\zeta^2 \sin^2 \tfrac{3}{2}\theta). \tag{9}$$

The variable ζ_0 plays no role in the phase transition. The exponents discussed above, which Griffiths calls the subsidiary tricritical exponents, are related to the exponents of the scaling function by

$$\begin{aligned} 2-\alpha &= 2-\alpha' = (2-\alpha_t)/\phi_t, \\ \beta &= (1-\alpha_t)/\phi_t, \\ \gamma &= \gamma' = \alpha_t/\phi_t, \\ \gamma'_\perp &= (2\Delta_t + \alpha_t - 2)/\phi_t; \end{aligned} \tag{10}$$

so that the low- and high-temperature exponents are the same.

This theory also predicts that at least close to the tricritical point the critical lines are described by $t = c\zeta^{\phi_t}$, where c is a constant, and $\theta = \pi/3, \pi$, or $5\pi/3$. Attempts to modify the theory by introducing a new exponent to characterize the approach of the critical lines to the zero field line do not alter the exponent relationships, except in the case of rather special assumptions about the structure of the scaling function—and even then the changes are in the wrong direction to explain table 1.

The scaling theory thus seems to imply that the anomalously low susceptibility exponent on the high-temperature side is an artifact of the analysis. Such an artifact might result from interference between the tricritical singularity and the Ising critical lines, which might not be well resolved by a short series. The point is that for finite ζ, the second ζ derivative of F_{sing} has a weak divergence at a temperature slightly above the tricritical point which will appear in the temperature series with an exponent α_I/ϕ_t (where α_I is the Ising specific heat exponent). This weak divergence may have been confused with the stronger true tricritical susceptibility divergence in the analysis.

6. Summary

The foregoing analysis indicates that the high- and low-temperature series have divergences in the same temperature range; and furthermore shows that there is a temperature in this range where the free energy and internal energy bridge continuously from low- to high-temperature behaviour. This may be evidence for a continuous phase transition, although a weak first-order phase transition is also possible. The resolution of these tests is unfortunately rather poor.

The critical exponents that have been calculated do not show the equality between high and low temperatures (for a given compliance) which is predicted by scaling theory. This, coupled with the anomalously low values of the high-temperature exponents, and consideration of the nature of the high-temperature, zero-field approach to the tricritical point, may indicate that the high-temperature series cannot be trusted.

Acknowledgments

I would like to thank Michael Fisher for his advice, and Doochul Kim for pointing out an error in one of my series.

Appendix. Low-temperature free energy series

The expansion of F in powers of x, y_1 and y_2 is given below. The notation y^n means $y_1^n+y_2^n$, and $y^m y^n$ is $y_1^m y_2^n + y_1^n y_2^m$.

$$\begin{aligned}-F/T = {} & yx^6+y^2(3x^{10}-3\tfrac{1}{2}x^{12})+yy(3x^{11}-3\tfrac{1}{2}x^{12})+y^3(15x^{14}-36x^{16}+21\tfrac{1}{3}x^{18}) \\ & +y^2y(30x^{15}-21x^{16}-72x^{17}+64x^{18})+y^4(3x^{16}+83x^{18}-328\tfrac{1}{2}x^{20} \\ & +405x^{22}-162\tfrac{3}{4}x^{24})+y^3y(12x^{18}+186x^{19}-117x^{20}-808x^{21}+567x^{22} \\ & +810x^{23}-651x^{24})+y^2y^2(6x^{18}+63x^{19}+40\tfrac{1}{2}x^{20}-423x^{21}-9x^{22} \\ & +810x^{23}-488\tfrac{1}{4}x^{24})+y^5(48x^{20}+426x^{22}-2804x^{24}+\ldots) \\ & +y^4y(48x^{21}+84x^{22}+1254x^{23}-917x^{24}+\ldots) \\ & +y^3y^2(144x^{22}+978x^{23}+357x^{24}+\ldots)+y^6(18x^{22}+486x^{24}+\ldots) \\ & +72y^5yx^{24}+36y^4y^2x^{24}+8y^7x^{24}+y^8x^{24}+\ldots .\end{aligned}$$

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