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Cayley tree approximation for the Potts model†

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Abstract. An approximation to the partition function of the standard Potts model is constructed by considering only the dominant tree-like configurations. This approximation gives a good representation of the positions of the non-physical singularities obtained from low-temperature series, and it is also possible to relate the behaviour of the approximations to the order of the Potts model transitions. It is found that for the two-dimensional lattices studied the transition is first-order for $q > 4$, whereas for the three-dimensional lattices it is first-order when $q > 2$.

1. Introduction

The question of the nature of the transition in the standard Potts model and how this depends on lattice dimensionality has proved extremely difficult to resolve. On the simple quadratic lattice Baxter (1973) has shown that the transition is continuous for a q-state model with $q \leqslant 4$. For three-dimensional lattices Kim and Joseph (1975) used a series method that indicates a first-order transition for $q = 3, 4 \ldots$. Unfortunately this method breaks down in two dimensions, so we cannot test its validity against the known results. Golner (1973) used a recursion technique on a continuous analogue of the Potts model and predicted a first-order transition for $q = 3$ in both two and three dimensions. An ϵ expansion by Amit and Shcherbakov (1974) indicated a first-order transition for $q = 3$ in three dimensions, but again the method cannot be compared with the known results for two dimensions. Series expansions using conventional methods of analysis are biased towards continuous transitions, but the results have been inconclusive (Ditzian and Oitmaa 1974, Enting 1974a, Ditzian 1974, Straley 1974). The mean-field approximation predicts a first-order transition for all dimensions, while a modified mean-field approximation (Alexander 1974) predicts a continuous transition for all dimensions.

In this situation any information which might help to elucidate the nature of the transition is welcome. We shall in the present paper generalize the approach which Domb and Guttmann (1970) used for the Ising model to the standard Potts model. These authors started from the low-temperature expansion for the logarithm of the partition function, $\ln Z$, in terms of weak lattice constants, and assumed that the dominant contribution is due to tree-like configurations for which the weightings of the lattice constants can be calculated exactly. For the Ising model ($q = 2$) this approximation provided a reasonable mimic of the true partition functions and a good approximation to the positions of non-physical and physical singularities for different lattices in

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two and three dimensions; it could not yield finer details of the transition like critical exponents. One might likewise hope that for the standard Potts model (general q) the approximation could provide a mimic for the partition function adequate to differentiate between a first-order and a continuous transition.

We have found that for $q > 2$ the approximate partition function gives a good representation of the non-physical singularities, except near the negative real axis. Apart from increasing our knowledge of the configurational properties of the model, a study of the non-physical singularities is important for series analysis. When studying the physical singularity the series can be transformed so that the non-physical singularities become less important (Guttmann and Thompson 1969, Guttmann *et al* 1970).

To obtain a reasonable value for the physical singularity needs more care since it is very sensitive to the value of lattice constant data. This was indicated by Domb and Guttmann (1970), who showed how by a small adjustment of a key parameter an understanding could be achieved of the structure of the physical singularity near the Curie point. A more detailed discussion, including an assessment of the effect of compact lattice constants, is given in a recent paper by one of us (Domb 1975). When $q > 2$ we find that we are able to interpret the behaviour of the order of the transition as a function of q and lattice dimension.

The basic calculations are given in § 2. Section 3 discusses the non-physical singularities and compares the approximate predictions with the results of series analysis. Section 4 studies the behaviour of the physical singularity and shows how the results can be interpreted to predict the order of the transition.

2. Approximate partition function

The Potts model that we consider has each site in one of q possible states, and an energy 0 for each neighbour pair in like states and J for each neighbour pair in unlike states. There is a field energy h for each site not in state 1.

For a one-dimensional chain we construct the transfer matrix $\mathbf{V}$:

$$\mathbf{V} = \begin{bmatrix} 1 & \eta u & \eta u & \dots & \eta u \\ \eta u & \eta^2 & \eta^2 u & \dots & \eta^2 u \\ \eta u & \eta^2 u & \eta^2 & \dots & \eta^2 u \\ \vdots & \vdots & & & \\ \eta u & \eta^2 u & & \dots & \eta^2 \end{bmatrix} \tag{1}$$

where

$$u = \exp(-\beta J) \tag{2}$$

$$\eta = \exp(-\beta h/2). \tag{3}$$

In zero field the eigenvalues have been obtained by Potts (1952) (see also Domb 1974).

To calculate the determinant of $\mathbf{V} - \lambda\mathbf{I}$ we perform the following operations that leave the determinant unchanged. Subtract row 2 from rows 3 to q; add columns 3 to q to column 2; this gives

$$\det(\mathbf{V}-\lambda\mathbf{I}) = [\eta^2(1-u)-\lambda]^{q-2}\begin{vmatrix} 1-\lambda & \eta(q-1)u \\ \eta u & \eta^2[1+(q-2)u]-\lambda \end{vmatrix}. \tag{4}$$

In regions of physical interest the largest eigenvalue is

$$\lambda_1 = \tfrac{1}{2}(1+\eta^2[(q-2)u+1]+[[\{1-\eta^2[(q-2)u+1]\}^2+4(q-1)\eta^2u^2]]^{1/2}); \quad (5)$$

the second largest is (in most regions)

$$\lambda_2 = \tfrac{1}{2}(1+\eta^2[(q-2)u+1]-[[\{1-\eta^2[(q-2)u+1]\}^2+4(q-1)\eta^2u^2]]^{1/2}). \quad (6)$$

The other eigenvalues are

$$\lambda_3 = \lambda_4 = \lambda_q = \eta^2(1-u). \quad (7)$$

These eigenvalues can be used to construct an approximate partition function for other lattices.

The method is a simple generalization of the method used by Domb and Guttmann (1970) and is based on approximating a weak graph expansion for the high-density partition function:

$$\ln Z = \sum_{\substack{\text{weak}\\ \text{graphs}}} p_G f_G(\mu, u) \sum_l \frac{v^l}{l^g}\left(\frac{\lambda_x}{\lambda_y}\right)^l. \quad (8)$$

The assumption made is that the behaviour is dominated by the contributions fron Cayley trees. The $f_G(\mu, u)$ for Cayley trees of l sites is approximated by $(\lambda_x/\lambda_y)^l$ where $|\lambda_y| > |\lambda_x| \gg |$other eigenvalues of $\mathbf{V}|$. The field term of $\mathbf{V}$ is re-intepreted to allow for interaction of sites in the tree with unperturbed sites outside the Cayley tree so that

$$\eta^2 = u^{z-2}\mu \quad (9)$$

$$\mu = \exp(-\beta H) \quad (10)$$

where the lattice has coordination number z and field energy H for sites not in state 1. The sum over Cayley trees of l sites is approximated by an assumed dependence v^l/l^g. The constants v are estimated from the results of direct enumerations. For the square, triangular, SC, BCC, FCC lattices they have been given by Domb and Guttmann. Using a factor $1/z$ for convenience of scale we have estimated for additional lattices

$v/z \simeq 1{\cdot}45$ diamond

$v/z \simeq 1{\cdot}1$ honeycomb.

We begin by expanding the eigenvalues to leading order to that

$$\lambda_1 = 1 + \ldots \quad (11)$$

$$\lambda_2 = \eta^2[1+(q-2)u] + \ldots \quad (12)$$

$$\lambda_3 = \eta^2(1-u) + \ldots. \quad (13)$$

To this order we have $|\lambda_1| > |\lambda_2| > |\lambda_3|$ for $\mu = 1$, only outside the circle of centre $u = (1-q)^{-1}$ and radius $(q-1)^{-1}$ in the complex plane. Since we really require $|\lambda_2| \gg |\lambda_3|$ this estimate provides only a rough indication of the region in which the approximations break down. The fact that $|\lambda_2| \simeq |\lambda_3|$ near the boundaries of this circle means that using λ_3/λ_1 in (8) is not likely to give a particularly accurate representation of $\ln Z$ near $u = (1-q)^{-1}$.

The singularities of (8) are expected at

$$\lambda_2/\lambda_1 = 1/v. \quad (14)$$

Using (8) and (9) we obtain as a first estimate

$$1/v \simeq u^{z-2}[1+(q-2)u]. \tag{15}$$

We refer to this as approximation I. The results are tabulated in table 1.

For $q = 2$ the spin $\frac{1}{2}$ Ising model approximation I predicts singularities equally spaced on a circle centred on the origin and, as pointed out by Domb and Guttmann, this provides a rather crude estimate to the true behaviour. The results shown in table 1 show that approximation I improves with increasing q. Using the full expressions for λ_1, λ_2, equation (14) leads to

$$v-(1+v^2)\mu u^{z-2}[1+(q-2)u]+(1+v)^2\mu u^z(q-1)+v\mu^2u^{2z-4}[1+(q-2)u]^2 = 0. \tag{16}$$

We refer to this as approximation II and give the results in table 1 for $\mu = 1$.

Table 1. Comparison of approximation estimates of singularities with results from series expansions. The real positive roots of two-dimensional models are known exactly. Estimates for FCC and SC, $q = 3$, are obtained from earlier work using high-temperature expansions. Because of the probability of first-order transitions the estimates of the transition temperature in three dimensions are only approximate. Estimates of the non-physical singularities are obtained from Padé approximants to the logarithmic derivative of the spontaneous order.

Lattice	v	q	Series/Exact	Approximation I (equation (15))	Approximation II (equation (16))
FCC	23·8	3	0·77	0·691	0·885
			0·54 ± 0·44i	0·57 ± 0·39i	0·55 ± 0·44i
			0·20 ± 0·66i	0·24 ± 0·66i	0·21 ± 0·65i
			−0·17 ± 0·67i	−0·17 ± 0·70i	−0·17 ± 0·66i
			−0·51 ± 0·48i	−0·57 ± 0·50i	−0·51 ± 0·48i
			−0·69 ± 0·20i	−0·92 ± 0·05i	−0·71 ± 0·17i
Triangular	8·4	3	0·532	0·528	0·69 ± 0·07i
			0·02 ± 0·52i	0·07 ± 0·55i	0·03 ± 0·51i
			−0·4 ± 0·4i	−0·83 ± 0·16i	−0·54 ± 0·25i
BCC	15·2	3	0·68	0·588	0·695
			0·28 ± 0·51i	0·33 ± 0·50i	0·28 ± 0·51i
			−0·23 ± 0·53i	−0·26 ± 0·59i	−0·23 ± 0·53i
			−0·58 ± 0·21i	−0·86 ± 0·73i	−0·61 ± 0·21i
Diamond	5·8	3	∼0·4	0·36	0·44
			∼ −0·39 ± 0·25i	−0·68 ± 0·15i	−0·38 ± 0·24i
Square	5·06	3	0·366	0·356	0·52 ± 0·06i
			−0·32 ± 0·29i	−0·68 ± 0·15i	−0·38 ± 0·25i
		4	$\frac{1}{3}$	0·323	0·46
			−0·26 ± 0·27i	−0·41 ± 0·31i	−0·31 ± 0·25i
		5	0·309	0·300	0·400
			−0·23 ± 0·25i	−0·31 ± 0·30i	−0·27 ± 0·24i
SC	10·5	3	0·586	0·501	0·606
			0·03 ± 0·49i	0·06 ± 0·53i	0·03 ± 0·49i
			−0·50 ± 0·24i	−0·81 ± 0·10i	−0·53 ± 0·23i
		4	∼0·56	0·470	0·560
			0·04 ± 0·49i	0·09 ± 0·49i	0·05 ± 0·46i
			−0·49 ± 0·23i	−0·57 ± 0·28i	−0·46 ± 0·24i
		5	∼0·55	0·449	0·529
			0·03 ± 0·47i	−0·10 ± 0·46i	0·05 ± 0·44i
			−0·49 ± 0·22i	−0·49 ± 0·28i	−0·41 ± 0·23i

3. Location of non-physical singularities

Here we compare the location of the non-physical singularities as estimated from series expansions with the locations of the complex roots of (15) and (16). We find that most of the singularities are predicted by equation (16) with an accuracy comparable to the accuracy with which estimates can be obtained from series. This is not true for singularities near the negative real axis since in this region $|\lambda_2| \simeq |\lambda_3|$.

The estimated positions of the singularities depend slightly on which function is analysed. The results given in table 1 are obtained from Padé approximants to the logarithmic derivative of the spontaneous order since these series gave the most regular estimates.

The low-temperature series for $q = 3$ are known to u^{17} on the triangular lattice and u^{47} on the FCC lattice (Enting 1974a). The method of partial generating functions (Enting 1974b) has been used to give series to u^{37} on the BCC, u^{15} on the diamond and u^{10} on the honeycomb lattice. For general q Straley and Fisher (1973) give square lattice series to u^{13} and Straley (1974) gives SC lattice series to u^{24}. The zero-field partition function series of Kihara *et al* (1954) (to u^{16} on the square lattice) have not been used here. We have not considered the honeycomb lattice because it is a special case, the low-temperature honeycomb partition function corresponding to the high-temperature triangular partition function by a duality relation. Since the triangular lattice three-state Potts model with antiferromagnetic interaction has a unique ground state, we can expect an order–disorder transition on the triangular lattice for a negative value of the high-temperature expansion variable. (The solution of Kim and Joseph (1974) has a root at $x \simeq -0{\cdot}8$ where x is the high-temperature expansion variable $(1-u)/[1+(q-1)u]$.) By duality this should give a root near $-0{\cdot}8$ on the negative u axis for the honeycomb lattice. This special system will be considered elsewhere.

Equation (15) (approximation I) gives $z-1$ roots on a roughly circular arrangement around the origin. There are also $z-1$ roots of equation (16) (approximation II) in a similar pattern around the origin. The exceptions are for $q = 2$, z even, when the correct expansion variable is u^2 and $\frac{1}{2}z-1$ roots occur.

The results given in table 1 show that there is a slight improvement in approximation II as q increases. The results near the negative real axis are always rather poor, which is to be expected since $|\lambda_2| \simeq |\lambda_3|$. For most lattices all the non-physical singularities are on or near the negative axis for $q = 2$, so we cannot make valid comparisons between $q = 2$ and $q = 3$. The exception is the FCC lattice which has a pair of singularities with $\mathrm{Re}(u) > 0$ for $q = 2$. Domb and Guttmann found $u = 0{\cdot}074 \pm 0{\cdot}533\mathrm{i}$ from series and $0{\cdot}105 \pm 0{\cdot}516\mathrm{i}$ from their approximation. For high values of q we find better agreement, except near the negative real axis.

4. Physical singularity

In § 2 we obtained equation (16) whose roots correspond approximately to the singularities of the Potts model. When examining the roots we find that there are no positive roots for $q < 4$ in two dimensions and $q < 2$ in three dimensions. Since these ranges are those in which continuous transitions are expected, we examine the behaviour more closely. Since the left-hand side of (16) is positive for $u = 0$ and positive for large u, there will be an even number of roots for $u > 0$. The dividing case between two roots

and no roots is the double root given by

$$\frac{\partial v}{\partial u} = 0 \tag{17}$$

whence

$$(z-2)+(q-2)(z-1)u-z(q-1)u^2-(z-2)u^{z-2}-(q-2)(2z-3)u^{z-1}-(q-2)^2(z-1)u^z$$
$$+(q-1)(z-4)u^z-(q-2)(q-1)(z-2)u^{z+1}=0. \tag{18}$$

For any given q the u value can be substituted into (14) to give v. Equation (18) corresponds to equation (17) of Domb and Guttman (1970) who referred to this limiting value of v as v^*. Equations (14) and (18) serve to define $v^*(q, z)$. We have plotted $v^*(q, z)/z$ for $z = 3$, 4, 6, 8, 12 and $1{\cdot}8 < q < 6$ in figure 1. (It should be noted that $v^*(2, 8) \simeq 14{\cdot}8$ and not 15·6 as given by Domb and Guttmann.)

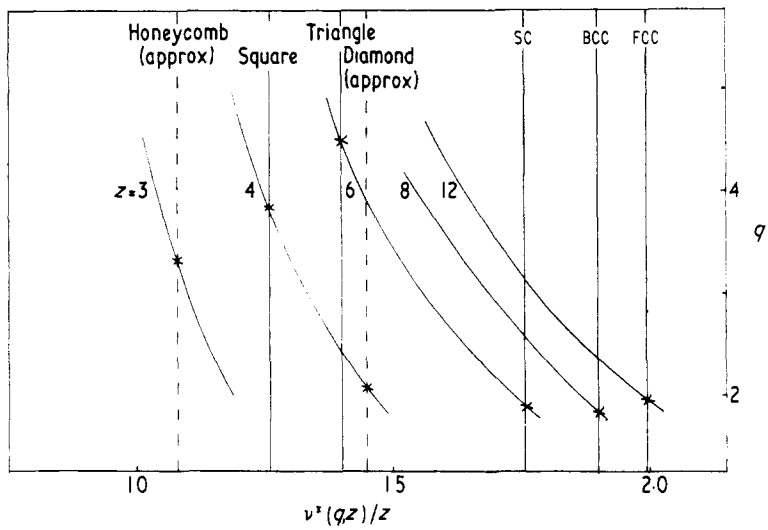

Figure 1. A plot of $v^*(q, z)/z$ against q for various z values. The denominator z is purely for convenience in plotting the graph. Values of v/z for actual lattices are shown (vertical lines) The intersections with the appropriate v^* lines are shown as crosses. These intersections occur for $q \simeq 4$ in two dimensions and $q \simeq 2$ in three dimensions.

The vertical lines on figure 1 give the v/z values for various lattices, so the intersections with the $v^*(q, z)/z$ lines, for appropriate z, give q values below which there are no roots on the positive axis.

To interpret the behaviour of $v^*(q, z)$ in terms of the order of the transition we return to equations (5), (6) and (14) and consider μ values other than 1. The general behaviour in the μ–u plane is shown in figure 2. The line of singularities is the approximation to the spinodal curve. For the case $v > v^*$ shown in figure 2(*b*) the spinodal curve crosses the u axis. Kim and Joseph (1975) show how this type of behaviour can be expected to correspond to a first-order transtion in zero field. Presumably the line of first-order transitions continues until it terminates with a critical point at some positive field value. For $v < v^*$ as shown in figure 2(*a*), the approximate partition function does not predict any physical singularity in zero field. Since the behaviour of the Ising model ($q = 2$) is

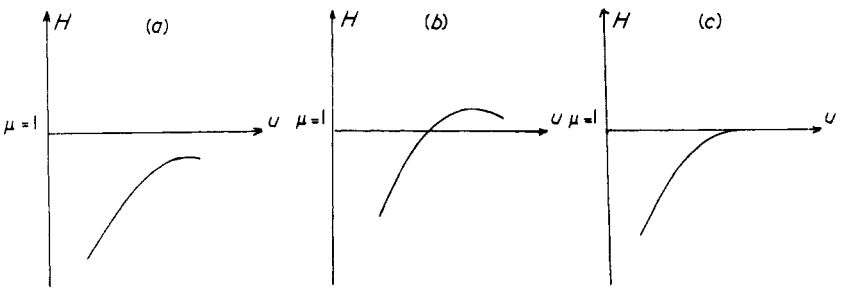

Figure 2. Behaviour of the spinodal curve from solution of (12) (*a*) $v < v^*$: equation (12) predicts that the spinodal curve will not cross the $H = 0$ line. We conjecture that the true spinodal curve extends to the u axis and that the transition is continuous; (*b*) $v > v^*$: the physically meaningful section of the spinodal curve cuts the u axis indicating a first-order transition, (*c*) $v = v^*$: since we have no detailed knowledge of the nature of the correction terms, using $v = v^*$ as the dividing case between first-order and continuous transitions is only approximate

well known, we can confidently predict a continuation of the spinodal curve to a continuous transition point on the u axis. As remarked above, $v = v^*$ (figure 2(*c*)) is observed to correspond to the boundary between first-order and continuous transitions. Since figure 2(*a*) clearly shows the importance of correction terms near the critical point, taking $v = v^*$ will give the division between first-order and continuous transitions only approximately.

5. Conclusions

We have seen that approximating the partition function of the standard Potts model by considering only contributions from Cayley trees gives a useful description of the model. Apart from representing the position of the non-physical singularities quite accurately, the approximation leads to a correlation between lattice properties and the order of the Potts model transition. The requirement $v < v^*(q, z)$ for a continuous transition shows how the combinatorial properties of the lattice relate to the types of critical behaviour. At the crudest level we can describe this phenomenon by noting that for a given value of the coordination number z, the value of v will increase with lattice dimensionality. It remains to be seen whether other lattices, such as the various second-neighbour lattices, will have behaviour that agrees with the pronounced dimension dependence shown in figure 1.

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