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Series expansions for the Potts model II. Partial generating functions in two dimensions

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Abstract. The formalism for obtaining high-field expansions for the Potts model by means of partial generating functions is discussed. The method is applied to the square and honeycomb lattices for small q values of the q-state standard Potts model. The critical isotherm is investigated.

1. Introduction

The work in this paper is aimed at formalizing and then extending the author's previous work on high-field expansions for the Potts model (Enting 1974, to be referred to as I).

The question that has aroused most interest in the Potts model is the order of the transition. Baxter (1973) has shown that for the square lattice the transition is continuous if q, the number of states, is less than or equal to four and is first order for greater than four states. In contrast, the mean-field approximation and the renormalization group work of Golner (1973) predict a first-order transition in the three-state model in two or three dimensions. A first-order transition for q equals three in three dimensions has been indicated by series analysis (Kim and Joseph 1974b, Ditzian and Oitmaa 1974). In contrast, a continuous transition is indicated by the series analysis work of Enting (1974), Ditzian (1974) and Straley (1974). In the present work we consider developing series in terms of partial generating functions expressed as codes. In three dimensions this technique is applicable to the body-centred cubic (BCC), simple cubic (SC) and diamond lattices. At present the only series available are for $q = 3$ on SC, BCC and face-centred cubic (FCC) (five high-field polynomials are given in I) and terms up to order 24 in the temperature grouping given by Straley for general q on the SC lattice. The actual series calculated and analysed in the present work are for two dimensions and small q values. Effective utilization of low-temperature series on three-dimensional lattices must await further information on the location and character of the transitions.

In § 2 we discuss high-field expansions in terms of linkage rules of the type given by Sykes and Gaunt (1973a). Section 3 then shows how the method of partial generating functions (Sykes *et al* 1965) is generalized to the q-state Potts model. A brief account of this work was given in I. This technique enables us to interpret graphically the fact that the star-triangle transformation is valid only at the transition (Stephen and Mittag 1972). In § 4 we investigate the critical isotherm for square and honeycomb lattices. Section 5 gives additional terms in the temperature grouping. The coded expressions for partial generating functions and the high-field polynomials for the three-state system on the honeycomb lattice are given in the appendix.

2. High-field expansions

In this section we expand the outline of the method given in I. The most important concept is that of the 'linkage rule'. This concept was introduced by Sykes and Gaunt (1973a) to discuss high-field expansions for the general spin Ising model.

The example given in equations (2) to (4) is for the three-state Potts model, but the other expressions refer to the q-state model in which the energy is zero if two interacting sites are in the same state and J otherwise. We consider only nearest-neighbour interactions.

High-field expansions for the configurational free energy are perturbation expansions about a fully aligned state which will be the zero of energy according to the definition above.

The expansion is

$$\ln \Lambda = \ln \sum_{\text{all perturbations}} \exp(-\beta \,.\text{Energy}). \tag{1}$$

For the three-state (a, b, c) Potts model the energy is

$$E = h_1 N_a + h_2 N_b + J(N_{ac} + N_{bc} + N_{ab}). \tag{2}$$

In I general values of the fields h_1, h_2 were allowed, but the present work is confined to the case of $h_1 = h_2 = h$.

If we are expanding about the c state, the graphical formulation of the expansion is simplified if we eliminate N_{ac}, N_{bc} from (2) using

$$zN_a = 2N_{aa} + N_{ab} + N_{ac} \tag{3a}$$

$$zN_b = 2N_{bb} + N_{ab} + N_{bc} \tag{3b}$$

to give

$$E = h(N_a + N_b) + J(zN_a + zN_b - 2N_{aa} - 2N_{bb} - N_{ab}) \tag{4}$$

z is the lattice coordination number. This is a linkage rule of the type described by Sykes and Gaunt (1973a).

An investigation of the sum over all perturbations shows how the expansion can be represented as a problem in decorating strong graphs

$$\sum_{\text{all perturbations}} \exp(-\beta E) = \sum_{n} \sum_{\substack{\text{all topologically} \\ \text{distinct arrangements} \\ \text{of } n \text{ sites}}} \sum_{\substack{\text{all embedding of} \\ \text{this topology}}} \sum_{\substack{\text{all } 2^n \text{ arrangements} \\ \text{of } a, b \text{ spins on the} \\ n \text{ sites}}} \exp(-\beta E). \tag{5}$$

In this context 'topologically distinct' is required to distinguish between different values of the E function summed over all arrangements of a, b spins. If one represents the arrangement of the n sites by a strong graph the $\Sigma \exp(-\beta E)$ will depend on the adjacency matrix of the graph but not on how it is embedded on the lattice.

We may thus replace the first two summations in (5) by a sum over all graphs, and the third sum by including the strong lattice constant as a multiplicative factor. The last sum corresponds to summing over all ways of decorating the graph with a and b sites. On taking the logarithm we replace the lattice constant by the term in the lattice constant that is linear in the number of sites.

The linkage rule (4) means that we have

$$\ln \Lambda = \sum l_{mn} u^n \mu^m = \sum_m \mu^m L_m(u) \tag{6}$$

where

$$u = \exp(-\beta J)$$

$$\mu = \exp(-\beta h)$$

and $L_m(u)$ are polynomials of degree mz in u. All these arguments can be extended to linkage rules other than (4) and for general Ising spin have been discussed by Fox (1972) and Sykes and Gaunt (1973a).

For the q-state Potts model the interaction energy is

$$\begin{aligned} E &= J \sum_{i<j=1}^{q} N_{ij} \\ &= J \sum_{i<j=1}^{q-1} N_{ij} + \sum_{i=1}^{q-1} \left(zN_i - N_{ii} - \sum_{j=1}^{q-1} N_{ij} \right) \\ &= J \sum_{i=1}^{q-1} \left(zN_i - 2N_{ii} - \sum_{j=i+1}^{q-1} N_{ij} \right) \end{aligned} \tag{7}$$

using

$$zN_i = \sum_{j=1}^{q} N_{ij} + N_{ii} \tag{8}$$

to eliminate N_{iq} from the first line.

3. The method of partial generating functions

In this section we show how the method of partial generating functions developed by Sykes *et al* (1965) can be generalized to the Potts model. The principles have been described by Sykes and Gaunt (1973a).

We divide the lattice into two equivalent sublattices so that all the neighbour pairs lie one on each sublattice. We divide the $L_n(u)$ defined by (6) according to the number of perturbed sites on each sublattice so that $\bar{L}_{nm}$ is the sum of all perturbations with n spins on the A sublattice and m spins on the B sublattice.

Then

$$L_n(u) = \sum_m \bar{L}_{m,n-m}(u). \tag{9}$$

We will now show how to calculate $F_n(u, \mu)$ defined by

$$F_n(u, \mu) = \sum_{m=0}^{\infty} \mu^m u^{-zn} \bar{L}_{mn}(u) \tag{10}$$

and since

$$\bar{L}_{mn}(u) = \bar{L}_{nm}(u) \tag{11}$$

a knowledge of F_0 to F_M will give L_1 to L_{2M+1}.

There are several features of the calculation of the F_n that will prove to have important consequences.

(i) The expansions for each F_n can be expressed as a sum over a finite number of graphs on the B sublattice.

(ii) The graphs needed for the Potts model (or for any other multi-state system with more general nearest-neighbour interactions) are precisely the same graphs as for the $q = 2$ system, the spin $\frac{1}{2}$ Ising model. This means that no additional graph counting is needed but that as in § 2 we are concerned with a graph decoration problem.

(iii) The decorated graphs give contributions to F_n which can be described by a linkage rule analogous to those in § 2. This property is also true for the spin $\frac{1}{2}$ Ising model and it is possible to represent relations between two distinct systems by relating the linkage rule of $L_n(u)$ for one to the linkage rule of $F_n(u, 1)$ for the other. Examples of this type of relation can be found in Gaunt (1974) and in Sykes and Gaunt (1973b) where the relation between the two systems is the star-triangle transformation. The work below generalizes this relation to general q.

In each of the F_n we are considering n perturbed sites on the B sublattice and have to sum over all possible perturbations of sites on the A sublattice. For A sites neighbour to one or more B sites, the contributions to F_n will depend on the configuration of the B sites according to the linkage rules described below. In any case the summation is over a finite number of possible perturbations and in principle presents no problems.

There are however an infinite number of A sites that are not neighbour to perturbed B sites and which therefore have a contribution to F_n given by an infinite sum. If the appropriate combinatorial factor for m perturbed A sites not neighbour to any of a particular configuration of n B sites is g_m, then the sum over all perturbations of the disconnected A sites is

$$\sum_n g_n[(q-1)u^z\mu]^n.$$

This is a function of $(q-1)u^z\mu$ and so can be obtained from the $q = 2$ case by replacing $u^z\mu$ by $(q-1)u^z\mu$. This is because the g_n is the term of order N^0 in that lattice constant for n A sites not neighbour to the particular configuration of B sites (where N is the number of sublattice sites). Thus g_n is independent of q and we have

$$F_0 = \ln[1+(q-1)u^z\mu] = \ln f_1. \tag{12}$$

If we consider an A site neighbour to one perturbed B site then the sum over all possible perturbations of the A site is

$$f_2 = 1+u^{z-2}\mu+(q-2)u^{z-1}\mu \tag{13}$$

where the terms correspond respectively to

(i) the A site unperturbed,

(ii) the A site perturbed into the same state as the B site,

(iii) the A site perturbed into each of the $(q-2)$ other states.

Each of the sums described by the f_i for $i \geqslant 2$ is finite and so of order N^0. The contribution to F_n is thus obtained by combining all the summations by multiplying the various f_i. As described above, the infinite summation over disjoint A sites is obtained from the $q = 2$ case by generalizing $u^z\mu$ to $(q-1)u^z\mu$. Since for $q = 2$ the contributions of the infinite sum to the F_n are in the form of negative powers of f_1, this will also be true for the general q-state model.

The other factors are

$$f_3 = 1+u^{z-4}\mu+(q-2)u^{z-2}\mu \tag{14}$$

for an A site adjacent to two B sites both perturbed into the same state.

$$f_4 = 1+2u^{z-3}\mu+(q-3)u^{z-2}\mu \tag{15}$$

for an A site adjacent to two B sites perturbed into different states.

$$f_5 = 1 + u^{z-6}\mu + (q-2)u^{z-3}\mu \tag{16}$$

for an A site neighbour to three B sites in the same perturbed state.

$$f_6 = 1 + u^{z-5}\mu + u^{z-4}\mu + (q-2)u^{z-3}\mu \tag{17}$$

for an A site with two B sites in one perturbed state and one in another perturbed state.

$$f_7 = 1 + 3u^{z-4}\mu + (q-4)u^{z-3}\mu \tag{18}$$

for an A site with three perturbed B neighbours in three different states.

For the lattices with coordination number four or greater, additional f_i are needed and have been given in I. For a lattice of coordination number z one has

$$F_1 = (q-1)(f_2/f_1)^z. \tag{19}$$

The $(q-1)$ factor comes from summing over all possible states of the B site.

The B sublattice of a square lattice is also a square lattice but it must be regarded as a square lattice with both first- and second-neighbour bonds. These bonds are different since two B sites connected by a nearest-neighbour bond will have two common A neighbours, while two B sites connected by a second-neighbour bond only have one common A neighbour.

The contributions to F_2 for the square lattice are:

(i) from disconnected B sites

$$-4{\cdot}5(q-1)^2 f_2^8/f_1^8$$

(ii) from sites connected by a second-neighbour bond

$$2(q-1)f_2^6 f_3/f_1^7 \qquad \text{(same B states)}$$

$$+2(q-1)(q-2)f_2^6 f_4/f_1^7 \qquad \text{(different B states)}$$

(iii) sites connected by a nearest-neighbour bond

$$2(q-1)f_2^4 f_3^2/f_1^6$$

$$+2(q-1)(q-2)f_2^4 f_4^2/f_1^6.$$

For the honeycomb lattice the B sublattice is triangular. The contributions to F_2 are

$$-3\tfrac{1}{2}(q-1)^2 f_2^6/f_1^6 \qquad \text{(disconnected B sites)}$$

$$+3(q-1)f_2^4 f_3/f_1^5 \qquad \text{(connected B sites in same state)}$$

$$+3(q-1)(q-2)f_2^4 f_4/f_1^5 \qquad \text{(connected B sites in different states).}$$

The general term in the F_n is represented by the codes $(\lambda, \alpha, \beta, \gamma, \delta \ldots)$ which represent $f_1^{-\lambda} f_2^{\alpha} f_3^{\beta} f_4^{\gamma} f_5^{\delta} \ldots$ with

$$\lambda = \alpha + \beta + \gamma + \delta + \ldots. \tag{20}$$

In the appendix we quote F_3, F_4 for the 4, 5, 6-state system on the square lattice, and F_3, F_4 and F_5 for the 3-state system on the honeycomb lattice. (The expressions for $q = 3$ on the square lattice were given in I.)

For any particular set of perturbed B sites the contribution to the honeycomb F_n is for $q = 3$

$$(f_2/f_1)^{N_{ac}+N_{bc}}(f_3/f_1)^{N'_{aa}+N'_{bb}}(f_4/f_1)^{N'_{ab}}(f_5/f_1)^{N_{aaa}+N_{bbb}}(f_6/f_1)^{N_{aab}+N_{abb}}. \tag{21}$$

N_{aaa} etc are the number of significant triangles of perturbed sites (see Sykes *et al* 1965). The N'_{aa}, etc are numbers of bonds excluding the edges of significant triangles.

For the q-state Potts model on the honeycomb lattice we have from (6), (9), (10) for zero field

$$\begin{aligned}\ln \Lambda_{\mathrm{HC}} &= \sum_n F_n(u,1)u^{3n} \\ &= \ln[1+(q-1)u^3] + \sum_{G_n} g_n u^{3n} (f_2/f_1)^n (f_3/f_1 f_2^{\frac{2}{2}})^a (f_4/f_1 f_2^{\frac{2}{2}})^b \\ &\quad \times (f_5/f_1 f_2^{\frac{3}{2}})^c (f_6/f_1 f_2^{\frac{3}{2}})^d (f_7/f_1 f_2^{\frac{3}{2}})^e\end{aligned}$$

where Σ_{G_n} is the sum over all decorated strong graphs of n sites on a triangular lattice and g_n is the term linear in N in the lattice constant

$$a = \sum_i N'_{ii} \tag{23}$$

$$b = \sum_{i<j} N'_{ij} \tag{24}$$

$$c = \sum_i N_{iii} \tag{25}$$

$$d = \sum_{i \neq j} N_{iij} \tag{26}$$

$$e = \sum_{i<j<k} N_{ijk} \tag{27}$$

where N'_{ij}, N'_{ii} exclude bonds forming the edges of significant triangles. The summations cover $i, j, k = 1$ to $q-1$. Equation (8) has been used to include the f_2 contributions with other terms rather than treat it separately as in (21).

The types of vertices of a significant triangle completely specify the edges so that we have

$$N_{ii} = N'_{ii} + 3N_{iii} + \sum_{j \neq i} N_{iij} \tag{28}$$

$$N_{ij} = N'_{ij} + 2N_{iij} + 2N_{ijj} + \sum_{\substack{k,k \neq i \\ k \neq j}} N_{ijk}. \tag{29}$$

In terms of the N'_{ij} the linkage rule (7) becomes

$$\begin{aligned}E/J &= \sum_i zN_i - 2\sum_i N'_{ii} - 6\sum_i N_{iii} - 2\sum_i \sum_{j \neq i} N_{iij} - \sum_{i<j} \left(N'_{ij} + 2N_{iij} + 2N_{ijj} + \sum_{\substack{k \neq i \\ k \neq j}} N_{ijk} \right) \\ &= \sum_i zN_i - 2\sum_i N'_{ii} - \sum_{i<j} N'_{ij} - 6\sum_i N_{iii} - 4\sum_i \sum_{j \neq i} N_{iij} - 3\sum_{i<j<k} N_{ijk}.\end{aligned} \tag{30}$$

For the triangular lattice in zero field we have

$$\ln \Lambda_{\mathrm{tri}} = \sum_{G_n} g_n w^{6n} w^{-2a} w^{-6b} w^{-6c} w^{-4d} w^{-3e}. \tag{31}$$

So that we have a star–triangle relation connecting (31) to (22) by

$$\ln \Lambda_{\mathrm{tri}}(w) = \ln \Lambda_{\mathrm{HC}}(u) - \ln[1+(q-1)u^3] \tag{32}$$

if we can satisfy (33) to (38).

$$uf_1/f_2 = w^2 \tag{33}$$

$$f_3/f_1 f_2^2 = w^{-2} \tag{34}$$

$$f_4/f_1 f_2^2 = w^{-1} \tag{35}$$

$$f_5/f_1 f_2^3 = w^{-6} \tag{36}$$

$$f_6/f_1 f_2^3 = w^{-4} \tag{37}$$

$$f_7/f_1 f_2^3 = w^{-3}. \tag{38}$$

In actual fact for $\mu = 1, z = 3$ we have

$$f_3 = f_2/u \tag{39}$$

$$f_5 = f_1/u^3 \tag{40}$$

$$f_6 = f_2/u^2 \tag{41}$$

$$f_7 = f_4/u \tag{42}$$

so that only two of the equations (33) to (38) are independent. Writing them explicitly,

$$\frac{3u+(q-3)u^2}{1+u+(q-2)u^2} = w \tag{43}$$

$$\frac{u+u^2+(q-2)u^3}{1+(q-1)u^3} = w^2. \tag{44}$$

The solution is given by

$$u^{-1} = 1+2h\sqrt{q} \tag{45}$$

where h is a solution of

$$8h^3-6h = \sqrt{q}. \tag{46}$$

The important property of this solution is that it also satisfies

$$u = \frac{1-w}{1+(q-2)w}. \tag{47}$$

The duality transformation for the honeycomb triangular system gives, for any $u < u_c$

$$\ln \Lambda_{HC}(u) = \ln \Lambda'_{tri}(u)+\ln[1+(q-1)u^3] \tag{48}$$

where $\ln \Lambda_{tri}$ is the high temperature form of the configurational free energy on the triangular lattice. Equation (47) is, however, precisely the relation connecting the high-temperature expansion variable to the low-temperature expansion variable, and so for u defined by (45) equations (32), (48) give

$$\ln \Lambda'_{tri}(u) = \ln \Lambda_{tri}(w) \tag{49}$$

and so the temperature at which the star–triangle transformation is valid is actually the transition temperature at which the high- and low-temperature expansions of the free energy are equal.

If one assumes that there is a unique transition temperature then it must have u_c given by (45).

The fact that the star–triangle transformation is valid only at the critical point was pointed out by Stephen and Mittag (1972), and the expressions (45), (46) have been previously given by Kim and Joseph (1974a).

4. Investigation of the critical isotherm

In this section we investigate the critical isotherm for the models whose code expansions are given in the appendix. The direct application of this analysis is in determining the critical exponent δ for continuous transitions and the critical magnetization for first-order transitions. An additional interest in the critical isotherm lies in the possibility of using the appropriate series to determine the type of transition. As indicated in the introduction, the order of the transition in three dimensions remains in doubt. Since the code method described in the previous section gives the full high-field polynomials, this may prove to be a particularly suitable method of investigating the behaviour in cases where high-temperature series have yielded a possible critical point. (The FCC lattice considered in I is a special case since one has a large number of terms in the temperature grouping but only a few in the field grouping.) In two dimensions we can use the exact results of Baxter (1973) to assess the validity of using series along the critical isotherm to determine the order of the transition. For this reason we apply all the methods for estimating δ and all the methods for estimating ψ_c to each of the series calculated, regardless of the order of transition expected.

To estimate δ the method used in I was to follow Gaunt and Sykes (1972) and construct the series for $-\mu(\mathrm{d}/\mathrm{d}\mu)\ln\psi$ at u_c. The reciprocals of the series coefficients should be estimates of δ and are tabulated in table 1.

Table 1. Estimates of δ. The estimates are reciprocals of series coefficients of $-\mu(\mathrm{d}/\mathrm{d}\mu)\ln\psi$.

(*a*) Square lattice

q \ n	4	5	6	7	8	9
3	15·87	16·24	15·59	15·86	15·54	15·56
4	17·25	17·64	16·91	17·20	16·83	16·86
5	18·96	19·45	18·68	19·05	18·68	19·05
6	20·89	21·56	20·79	21·29	20·94	21·07

(*b*) Honeycomb lattice

q \ n	6	7	8	9	10	11
3	16·59	16·01	16·00	16·34	15·92	15·71

For the $q = 3, q = 4$ state models on the square lattice the results seem to be consistent with $\delta = 15$. For $q = 6$ the value is much larger and slowly increasing. Since we have the exact result of Baxter (1973) that the transition is first-order for $q = 5$ and $q = 6$

we assume that the sequence of estimates for these cases must ultimately diverge but for $q = 6$, and even more for $q = 5$, this occurs very slowly and does not seem to be a reliable indication of the order of the transition. The use of this method to determine the order of the transition in three-dimensional systems would be even less reliable since there are no exact results for the critical temperature, and analysis of the critical isotherm would have to be based on an approximate series estimate. For the $q = 3$ model on the honeycomb lattice the estimates were again consistent with $\delta \simeq 15$, but the estimates had irregular oscillation. (This is possibly of period four, but we do not have sufficient terms to confirm this.)

Any method of analysis must make some assumptions about the behaviour of the function, ie the type of singularities expected. The most reasonable types of behaviour to postulate are:

(i) $\psi \sim (1-\mu)^{1/\delta}$

(ii) $\psi \sim (1-\mu)^{1/\delta'} + \psi_c$

or (iii) no singularities at $\mu = 1$.

We have analysed the series by using Padé approximants. Padé approximants to $(1-\mu)(\mathrm{d}/\mathrm{d}\mu) \ln \psi$ evaluated at $\mu = 1$ should give estimates of δ^{-1}. We find the δ estimates:

$$\delta = 15{\cdot}2 \pm 0{\cdot}5 \qquad q = 3 \quad \text{SQ}$$

$$\delta = 15{\cdot}8 \pm 0{\cdot}8 \qquad q = 4 \quad \text{SQ}$$

$$\delta = 18{\cdot}5 \pm 1{\cdot}0 \qquad q = 5 \quad \text{SQ}$$

$$\delta = 21{\cdot}1 \pm 1{\cdot}0 \qquad q = 6 \quad \text{SQ}$$

$$\delta = 15{\cdot}5 \pm 0{\cdot}7 \qquad q = 3 \quad \text{HC}.$$

If we assume the form (ii) which corresponds to a first-order transition then we can estimate δ' by constructing $(1-\mu)(\mathrm{d}/\mathrm{d}\mu) \ln(\mathrm{d}\psi/\mathrm{d}\mu)$ which evaluated at 1 gives estimates of $1/\delta' - 1$ (or $1/\delta - 1$ for the case (i) which is $\mu_c = 0$).

The estimates obtained were

$$1 - \frac{1}{\delta'} = 1{\cdot}00 \pm 0{\cdot}06 \qquad q = 3 \quad \text{SQ}$$

$$1 - \frac{1}{\delta'} = 1{\cdot}05 \pm 0{\cdot}10 \qquad q = 4 \quad \text{SQ}$$

$$1 - \frac{1}{\delta'} = 1{\cdot}0 \pm 0{\cdot}1 \qquad q = 5 \quad \text{SQ}$$

$$1 - \frac{1}{\delta'} = 1{\cdot}05 \pm 0{\cdot}1 \qquad q = 6 \quad \text{SQ}$$

$$1 - \frac{1}{\delta'} = 1{\cdot}00 \pm 0{\cdot}15 \qquad q = 3 \quad \text{HC}.$$

Since these δ' estimates cover a range that includes both a cusp and a negative divergence in ψ they do not reveal any useful information about the behaviour of the singularity.

Because of the rapid variation in ψ near $\mu = 1$ it is impossible to extrapolate ψ directly to estimate ψ_c. The variation would however be slower if ψ were raised to some

large power. We construct ψ^{15} and evaluate Padé approximants at $\mu = 1$. The estimates are

$$\psi_c^{15} = 0{\cdot}0050 \pm 0{\cdot}0005 \qquad q = 3 \quad \text{SQ}$$
$$\psi_c^{15} = 0{\cdot}018 \pm 0{\cdot}002 \qquad q = 4 \quad \text{SQ}$$
$$\psi_c^{15} = 0{\cdot}037 \pm 0{\cdot}010 \qquad q = 5 \quad \text{SQ}$$
$$\psi_c^{15} = 0{\cdot}063 \pm 0{\cdot}010 \qquad q = 6 \quad \text{SQ}.$$

Since for the $q = 3, q = 4$ cases these results are inconsistent with the Baxter result of a continuous transition, we are forced to conclude that Padé approximants have not been able to estimate ψ_c and nor do they indicate $\psi_c = 0$, even in the cases for which we believe that we know δ. The overall conclusion must be that analysis of the critical isotherm is not a useful means of determining the order of the transition. The major difficulty is associated with the rapid variation corresponding to small values of $1/\delta$. When investigating the spontaneous magnetization the small values of β will give similar difficulties.

5. The temperature grouping

We briefly point out that it is very easy to add to the honeycomb lattice series the terms

$$(q-1)(13\tfrac{1}{2}u^{10}\mu^{14} + 67\tfrac{1}{2}u^{10}\mu^{12} + u^9\mu^{13}).$$

These terms together with the polynomials L_1 to L_{11}, obtained by expanding F_0 to F_5, give the temperature grouping of the honeycomb lattice through to u^{10}.

These terms are obtained by generalizing the corresponding spin $\frac{1}{2}$ Ising model series by including the $(q-1)$ factor which is one for the spin $\frac{1}{2}$ Ising case. All these terms come from connected graphs and so the only 'decorations' that give the same order in u as the $q = 2$ case will be those decorations in which all perturbed sites are in the same state. Any decorations with several types of perturbed site will give terms of higher order in u. The $u^9\mu^{13}$ term has its graph formed of three hexagons with a common vertex (and three common edges). It can readily be seen that no decorations of this graph give terms of order u^{10}, and so the additional terms given above do complete the temperature grouping to order u^{10}.

Similarly, it is possible to extend the temperature grouping on the FCC and triangular lattices to more terms than were given in I, merely by considering a small number of the graphs for the spin $\frac{1}{2}$ Ising model.

The square lattice series have been extended and it has been possible to obtain the field dependence of the coefficients given by Kihara *et al* (1954). The 14th, 15th and 16th order low-temperature polynomials are for $q = 3$

$$u^{14}(4\mu^{12} + 16\mu^{11} + 60\mu^{10} + 152\mu^9 + 352\mu^8 + 496\mu^7 + 368\mu^6 - 1212\mu^5 + 604\mu^4)$$
$$u^{15}(24\mu^{10} + 160\mu^9 + 640\mu^8 + 1608\mu^7 + 2148\mu^6 - 4344\mu^5 + 944\mu^4)$$
$$u^{16}(2\mu^{16} + 12\mu^{15} + 44\mu^{14} + 136\mu^{13} + 334\mu^{12} + 716\mu^{11} + 1264\mu^{10} + 1982\mu^9 + 1788\mu^8 + 44\mu^7 - 5580\mu^6 + 2670\mu^5 - 836\mu^4).$$

Lower-order polynomials are given by Straley and Fisher (1973).

Analysis of the extended series gives

$$\beta = 0{\cdot}105 \pm 0{\cdot}005$$

$$\gamma' = 1{\cdot}45 \pm 0{\cdot}15.$$

These do not differ greatly from the estimates obtained by Straley and Fisher. They believed that they had underestimated γ' because their values violated the Rushbrooke inequality. In I we suggested that the result $\delta = 15$ implied that they had underestimated α' or β. Since the series for ψ seem to be the most regular and the β estimate is unchanged by taking longer series, it would appear that α' has been underestimated.

For other loose-packed lattices it is more appropriate to generalize the work of Sykes *et al* (1973). All the graphs for the general q-state code expansions are decorations of the $q = 2$ case and as explained above, the case in which all perturbed sites are in the same state will be the case that contributes the lowest power of u. For the $q = 2$ graphs Sykes *et al* have defined a number called the *class* of the code that gives the lowest power of u contributed by that code. To obtain all contributions to the temperature grouping up to some order, it is sufficient to consider all shadow lattice graphs that contribute at that order in the spin $\frac{1}{2}$ Ising model (selecting them by the class of their codes) and then to consider all decorations of these graphs.

There are two ways of reducing the work involved since the procedure described above is sufficient but not all necessary.

Firstly, as described by Sykes *et al* (1973), the work is reduced by ensuring that each contribution is obtained from the lowest F_n since most terms contributed to two distinct F_n.

Secondly, as remarked several times above, only the 'decorations' of the graphs that have all perturbed sites in the same state contribute at lowest order. It is therefore possible to exclude some decorated graphs from consideration. The most appropriate way of doing this is to generalize the concept of the class of a code to refer to decorated shadow lattice graphs.

6. Conclusions

The most immediate conclusions that can be drawn from this work concern the critical exponents. We can even attempt to estimate β for the three-state model on the honeycomb lattice. Padé approximants to $(u_c - u)(\mathrm{d}/\mathrm{d}u) \log \psi$ give

$$\beta = 0{\cdot}10 \pm 0{\cdot}01 \qquad q = 3 \quad \text{HC}.$$

This is based on terms to u^{10} and a knowledge of u_c. It should be noted that the Padé approximants to $(\mathrm{d}/\mathrm{d}u) \log \psi$ do not give particularly regular estimates of u_c. This is not surprising considering the shortness of the series, but it does mean that the result above should be treated with caution. Nevertheless, it is consistent with the estimate $\beta = 0{\cdot}105 \pm 0{\cdot}005$ (3-state SQ) obtained above, and is almost certainly less than $\beta = 0{\cdot}125$ for the $q = 2$ (spin $\frac{1}{2}$ Ising) case.

In contrast, it appears that in those cases where it is defined, ie if the transition is continuous, the exponent δ does not depend on the number of states, nor on the lattice, and is 15 in two dimensions.

Extrapolations of the estimates give

$$\delta = 15{\cdot}0 \pm 0{\cdot}4 \qquad q = 3 \quad \text{SQ}$$
$$\delta = 15{\cdot}8 \pm 0{\cdot}8 \qquad q = 4 \quad \text{SQ}$$
$$\delta = 15{\cdot}0 \pm 1{\cdot}5 \qquad q = 3 \quad \text{HC}.$$

The $q = 3$ case is in agreement with the $q = 2$ (spin $\frac{1}{2}$ Ising) value, but the $q = 4$ value is slightly higher. Looking at all the q values in table 1, if one assumes that the $q = 5$, $q = 6$ estimates ultimately diverge then it is apparent that as q increases, more terms are needed before limiting behaviour becomes apparent. It seems plausible that the $q = 4$ system does actually have $\delta = 15$ and that the apparent slight dependence on q is spurious.

While we believe that it is possible to estimate δ if the transition is known to be continuous, it has not been possible to find estimates for the discontinuity in ψ, nor have any of the methods of series analysis indicated a reliable way of determining the order of the transition. The only possibility is to assume δ is independent of q, and to regard any case that has δ estimates inconsistent with the $q = 2$ values as being first order. Results like the $q = 4$ case described here would have to be regarded as inconclusive in the absence of any other information about the type of transition. The only encouraging aspect is that as pointed out in § 4, many of the difficulties are associated with the small values of δ^{-1} (or of β if the spontaneous order is considered). Both β and δ^{-1} are expected to increase with increasing dimensionality, and so the difficulties may be somewhat diminished, but any such analysis must be based on pre-existing estimates of the transition temperature.

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Appendix

A.1. Code expansions for standard Potts model

(General expansions for F_0, F_1, F_2 are given in the text. For the square lattice the three-state codes are given in I.)

4 state, square lattice

$$\begin{aligned} F_3 = {} & 24(8,4,0,4)+24(8,4,2,2)+6(8,4,4)+24(8,5,0,2,0,0,1)+24(8,5,0,2,0,1) \\ & +48(8,5,1,1,0,1)+12(8,5,2,0,1)-504(11,10,0,1)-252(11,10,1) \\ & +48(9,6,1,2)+96(9,6,0,3)+48(9,6,2,1)+24(9,6,3)+72(10,8,1,1) \\ & -360(10,8,0,2)-198(10,8,2)+873(12,12) \end{aligned}$$

$$F_4 = 10260(14,12,0,2) - 5400(14,12,1,1) + 6480(14,12,2) + 432(12,8,3,1)$$
$$- 1314(12,8,0,4) + 888(12,8,1,3) - 1512(12,8,2,2) - 438(12,8,4)$$
$$- 7056(13,10,0,3) - 3096(13,10,1,2) - 3420(13,10,2,1)$$
$$- 1818(13,10,3) + 96(11,6,4,1) + 384(11,6,0,5) + 384(11,6,2,3)$$
$$+ 192(11,6,1,4) + 192(11,6,3,2) + 48(11,6,5) + 48(10,6,0,2,0,0,2)$$
$$+ 96(10,6,0,2,0,1,1) + 144(10,6,0,2,0,2) + 96(10,6,1,1,0,1,1)$$
$$+ 48(10,6,2,0,0,2) + 96(10,6,1,1,0,2) + 96(10,6,1,1,1,1)$$
$$+ 24(10,6,2,0,2) - 1080(12,9,0,2,0,0,1) - 1080(12,9,0,2,0,1)$$
$$- 2160(12,9,1,1,0,1) - 540(12,9,2,0,1) + 48(10,5,2,2,0,0,1)$$
$$+ 96(10,5,0,4,0,0,1) + 96(10,5,0,4,0,1) + 48(10,5,2,2,0,1)$$
$$+ 96(10,5,3,1,0,1) + 192(10,5,1,3,0,1) + 48(10,5,2,2,1)$$
$$+ 24(10,5,4,0,1) + 48(10,4,0,6) + 72(10,4,2,4) + 36(10,4,4,2)$$
$$+ 6(10,4,6) + 19548(15,14,0,1) + 9774(15,14,1)$$
$$+ 12(9,4,0,4,0,0,0,0,0,0,1) + 6(9,4,0,4,0,0,0,0,0,1)$$
$$+ 24(9,4,1,3,0,0,0,0,0,0,1) + 12(9,4,2,2,0,0,0,0,0,1)$$
$$+ 24(9,4,2,2,0,0,0,0,1) + 3(9,4,4,0,0,0,0,1) + 120(11,7,1,2,0,0,1)$$
$$+ 240(11,7,0,3,0,0,1) + 240(11,7,0,3,0,1) + 240(11,7,2,1,0,1)$$
$$+ 600(11,7,1,2,0,1) + 120(11,7,2,1,1,) + 60(11,7,3,0,1)$$
$$- 229432\tfrac{1}{2}(16,16).$$

5 state, square lattice

$$F_3 = 72(8,4,0,4) + 48(8,4,2,2) + 8(8,4,4) + 96(8,5,0,2,0,0,1) + 48(8,5,0,2,0,1)$$
$$+ 96(8,5,1,1,0,1) + 16(8,5,2,0,1) - 1344(11,10,0,1) - 448(11,10,1)$$
$$+ 96(9,6,1,2) + 288(9,6,0,3) + 96(9,6,2,1) + 32(9,6,3) + 144(10,8,1,1)$$
$$- 936(10,8,0,2) - 360(10,8,2) + 2069\tfrac{1}{3}(12,12)$$

$$F_4 = 34080(14,12,0,2) - 14400(14,12,1,1) + 16160(14,12,2) + 864(12,8,3,1)$$
$$- 4812(12,8,0,4) + 2688(12,8,1,3) - 4056(12,8,2,2) - 828(12,8,4)$$
$$- 28008(13,10,0,3) - 8040(13,10,1,2) - 9336(13,10,2,1)$$
$$- 3256(13,10,3) + 480(11,7,1,2,0,0,1) + 144(11,7,0,3,0,0,1)$$
$$+ 720(11,7,0,3,0,1) + 480(11,7,2,1,0,1) + 1680(11,7,1,2,0,1)$$
$$+ 240(11,7,2,1,1) + 80(11,7,3,0,1) + 192(11,6,4,1) + 1728(11,6,0,5)$$
$$+ 1152(11,6,2,3) + 576(11,6,1,4) + 384(11,6,3,2) + 64(11,6,5)$$
$$+ 384(10,6,0,2,0,0,2) + 384(10,6,0,2,0,1,1) + 384(10,6,1,1,0,1,1)$$

$$+192(10,6,1,1,0,2)+96(10,6,2,0,0,2)+192(10,6,1,1,1,1)$$
$$+32(10,6,2,0,2)+384(10,6,0,2,0,2)-5760(12,9,0,2,0,0,1)$$
$$-2880(12,9,0,2,0,1)-5760(12,9,1,1,0,1)-960(12,9,2,0,1)$$
$$+192(10,5,2,2,0,0,1)+576(10,5,0,4,0,0,1)+288(10,5,0,4,0,1)$$
$$+96(10,5,2,2,0,1)+192(10,5,3,1,0,1)+576(10,5,1,3,0,1)$$
$$+96(10,5,2,2,1)+32(10,5,4,0,1)+216(10,4,0,6)+216(10,4,2,4)$$
$$+72(10,4,4,2)+8(10,4,6)+69504(15,14,0,1)+23168(15,14,1)$$
$$+24(9,4,0,4,0,0,0,0,0,0,1)+48(9,4,0,4,0,0,0,0,0,0,1)$$
$$+12(9,4,0,4,0,0,0,0,0,1)+96(9,4,1,3,0,0,0,0,0,1)$$
$$+24(9,4,2,2,0,0,0,0,0,1)+48(9,4,2,2,0,0,0,0,1)$$
$$+4(9,4,4,0,0,0,0,1)-72512(16,16).$$

6 state, square lattice

$$F_3 = 160(8,4,0,4)+80(8,4,2,2)+10(8,4,4)+240(8,5,0,2,0,0,1)+80(8,5,0,2,0,1)$$
$$+160(8,5,1,1,0,1)+20(8,5,2,0,1)-2800(11,10,0,1)-700(11,10,1)$$
$$+160(9,6,1,2)+640(9,6,0,3)+40(9,6,3)+160(9,6,2,1)$$
$$+240(10,8,1,1)-1920(10,8,0,2)-570(10,8,2)+4041\tfrac{2}{3}(12,12)$$

$$F_4 = 85000(14,12,0,2)-30000(14,12,1,1)+32500(14,12,2)+1440(12,8,3,1)$$
$$-12620(12,8,0,4)+6000(12,8,1,3)-8480(12,8,2,2)-1340(12,8,4)$$
$$-77440(13,10,0,3)-16480(13,10,1,2)-19720(13,10,2,1)$$
$$-5110(13,10,3)+1200(11,7,1,2,0,0,1)+4800(11,7,0,3,0,0,1)$$
$$+1600(11,7,0,3,0,1)+800(11,7,2,1,0,1)+3600(11,7,1,2,0,1)$$
$$+400(11,7,2,1,1)+100(11,7,3,0,1)+320(11,6,4,1)+5120(11,6,0,5)$$
$$+2560(11,6,2,3)+1280(11,6,1,4)+640(11,6,3,2)+80(11,6,5)$$
$$+1440(10,6,0,2,0,0,2)+960(10,6,0,2,0,1,1)+800(10,6,0,2,0,2)$$
$$+960(10,6,1,1,0,1,1)+160(10,6,2,0,0,2)+320(10,6,1,1,0,2)$$
$$+320(10,6,1,1,1,1)+40(10,6,2,0,2)-18000(12,9,0,2,0,0,1)$$
$$-6000(12,9,0,2,0,1)-12000(12,9,1,1,0,1)-1500(12,9,2,0,1)$$
$$+480(10,5,2,2,0,0,1)+1920(10,5,0,4,0,0,1)+640(10,5,0,4,0,1)$$
$$+160(10,5,2,2,0,1)+320(10,5,3,1,0,1)+1280(10,5,1,3,0,1)$$
$$+160(10,5,2,2,1)+40(10,5,4,0,1)+640(10,4,0,6)$$
$$+480(10,4,2,4)+120(10,4,4,2)+10(10,4,6)+181000(15,14,0,1)$$
$$+45250(15,14,1)+120(9,4,0,4,0,0,0,0,0,0,0,1)$$

$$+120(9,4,0,4,0,0,0,0,0,0,1)+20(9,4,0,4,0,0,0,0,0,1)$$
$$+240(9,4,1,3,0,0,0,0,0,0,1)+40(9,4,2,2,0,0,0,0,0,1)$$
$$+80(9,4,2,2,0,0,0,1)+5(9,4,4,0,0,0,0,1)-177031\tfrac{1}{4}(16,16).$$

3 state, honeycomb

$$F_3 = 154\tfrac{2}{3}(9,9)-120(8,7,0,1)-120(8,7,1)+18(7,5,0,2)+36(7,5,1,1)+18(7,5,2)$$
$$+6(7,6,0,0,0,1)+2(7,6,0,0,1)+6(6,3,1,2)+2(6,3,3)$$

$$F_4 = -2076(12,12)+2304(11,10,0,1)+2304(11,10,1)-714(10,8,0,2)$$
$$-1428(10,8,1,1)-714(10,8,2)-144(10,9,0,0,0,1)-48(10,9,0,0,1)$$
$$+58(9,6,0,3)+30(9,6,1,2)+174(9,6,2,1)+10(9,6,3)$$
$$+36(9,7,1,0,0,1)+36(9,7,0,1,0,1)+12(9,7,0,1,1)+12(9,7,1,0,1)$$
$$+36(8,4,2,2)+36(8,4,1,3)+12(8,4,3,1)+12(8,4,4)+6(8,5,2,0,0,1)$$
$$+6(8,5,0,2,0,1)+24(8,5,1,1,0,1)+6(8,5,0,2,1)+6(8,5,2,0,1)$$

$$F_5 = 31078\tfrac{2}{3}(15,15)-44736(14,13,0,1)-44736(14,13,1)+21096(13,11,0,2)$$
$$+42192(13,11,1,1)+20196(13,11,2)-3728(12,9,0,3)-11184(12,9,2,1)$$
$$-8160(12,9,1,2)-2720(12,9,3,0)+3024(13,12,0,0,0,1)$$
$$+1008(13,12,0,0,1)+198(11,7,0,4)-864(11,7,1,3)-468(11,7,2,2)$$
$$+240(11,7,3,1)-354(11,7,4)-1656(12,10,0,1,0,1)$$
$$-1656(12,10,1,0,0,1)-552(12,10,0,1,1)-552(12,10,1,0,1)$$
$$+12(11,8,2,0,0,1)+12(11,8,0,2,0,1)-312(11,8,1,1,0,1)$$
$$-108(11,8,0,2,1)+120(11,8,1,1,1)-108(11,8,2,0,1)+180(10,5,1,4)$$
$$+360(10,5,2,3)+240(10,5,3,2)+120(10,5,4,1)+60(10,5,5)$$
$$+54(10,6,3,0,0,1)+36(10,6,0,3,0,1)+36(10,6,0,3,1)+54(10,6,1,2,1)$$
$$+234(10,6,1,2,0,1)+180(10,6,2,1,0,1)+36(10,6,2,1,1)$$
$$+42(10,6,3,0,1)+30(10,7,1,0,0,2)+24(10,7,0,1,0,2)$$
$$+24(10,7,0,1,1,1)+12(10,7,1,0,1,1)+6(10,7,1,0,2)+6(9,4,0,4,1)$$
$$+24(9,4,1,3,0,1)+12(9,4,2,2,1)+24(9,4,2,2,0,1)+24(9,4,3,1,0,1)$$
$$+6(9,4,4,0,1).$$

A.2. High-field polynomials, honeycomb, $q = 3$

$$L_1 = 2u^3$$
$$L_2 = 3u^4+3u^5-8u^6$$
$$L_3 = 6u^5+12u^6-30u^7-36u^8+50\tfrac{2}{3}u^9$$

$$L_4 = 14u^6+42u^7-93u^8-256u^9+273u^{10}+408u^{11}-392u^{12}$$

$$L_5 = 36u^7+144u^8-268u^9-1308u^{10}+888u^{11}+4124u^{12}-2352u^{13}-4656u^{14}+3398\tfrac{2}{5}u^{15}$$

$$L_6 = u^6+108u^8+465u^9-741u^{10}-5814u^{11}+1554u^{12}+26961u^{13}-3474u^{14}-59596u^{15}+18408u^{16}+53808u^{17}-31690\tfrac{2}{5}u^{18}$$

$$L_7 = 6u^7+6u^8+310u^9+1554u^{10}-2298u^{11}-23470u^{12}-3774u^{13}+143790u^{14}+52228u^{15}-461544u^{16}-89160u^{17}+813840u^{18}-113088u^{19}-629184u^{20}+310802\tfrac{2}{7}u^{21}$$

$$L_8 = 27u^8+54u^9+864u^{10}+5130u^{11}-7180u^{12}-92346u^{13}-47994u^{14}+672622u^{15}+618675u^{16}-2778492u^{17}-2225882u^{18}+7067160u^{19}+3116898u^{20}-10730560u^{21}+132384u^{22}+7431168u^{23}-3162560u^{24}$$

$$L_9 = 110u^9+330u^{10}+2388u^{11}+16244u^{12}-21960u^{13}-357096u^{14}-297748u^{15}+2950860u^{16}+4360866u^{17}-14135106u^{18}-22160256u^{19}+45418368u^{20}+56017240u^{21}-99859104u^{22}-67275744u^{23}+138023872u^{24}+12729216u^{25}-88509696u^{26}+33097272\tfrac{8}{9}u^{27}$$

$$L_{10} = 3u^8+459u^{10}+1671u^{11}+6616u^{12}+47463u^{13}-66786u^{14}-1349154u^{15}-1536897u^{16}+12483090u^{17}+25213819u^{18}-64777545u^{19}-161447984\tfrac{2}{5}u^{20}+233126871u^{21}+567553404u^{22}-643183500u^{23}-1153734288u^{24}+1318810425\tfrac{3}{5}u^{25}+1226520096u^{26}-1741158784u^{27}-324087552u^{28}+1061703168u^{29}-354124697\tfrac{3}{5}u^{30}$$

$$L_{11} = 24u^9+24u^{10}+1734u^{11}+7890u^{12}+17400u^{13}+122970u^{14}-216874u^{15}-4935384u^{16}-7223736u^{17}+51300972u^{18}+131439186u^{19}-277217502u^{20}-995456552u^{21}+990279138u^{22}+4389081426u^{23}-2908290236u^{24}-12210957360u^{25}+7748872032u^{26}+21223281984u^{27}-16296715392u^{28}-20454553728u^{29}+21598538240u^{30}+5977605120u^{31}-12812350464u^{32}+3857369274\tfrac{2}{11}u^{33}.$$

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