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The Potts model on Kagomé and honeycomb lattices

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Abstract. Low-temperature series have been derived for the q-state Potts model on the Kagomé lattice ($q = 3$ and 4) and for the 3-state honeycomb lattice. The series are derived by the finite-lattice method, with many additional terms obtained by noting the structure of the correction terms. Accurate estimates of the critical points are found, which confirm exact, but not rigorous results in the case of the honeycomb lattice, and refute previous conjectures in the case of the Kagomé lattice.

1. Introduction

The q-state Potts models [1] is one of the most important models in lattice statistical mechanics and contains the Ising model ($q = 2$) and bond percolation ($q = 1$ limit) as special cases. An excellent introduction to the Potts model, its properties, known results, and connections to many other problems can be found in Wu's classic review article [2]. Among the open problems, one of the most important remains the determination of the exact critical point on various two-dimensional lattices. The critical point for the Ising model can be found exactly for any two-dimensional lattice, but the generalization to the q-state Potts model is only known for the square, honeycomb, and triangular lattices [2, 3]. Even in these cases a rigorous derivation is often only possible for $q \geqslant 4$ and $q = 2$. The determination of the critical point for the Kagomé lattice has proved to be a particularly elusive problem [3–6].

In this paper we report on the derivation and analysis of low-temperature series for the 3-state honeycomb and 3- and 4-state Kagomé lattice Potts model. From the series we obtain estimates for the critical points, which for the honeycomb model confirms the validity of the exact but not rigorous result [7], and for the Kagomé lattice provides accurate results against which conjectures can be tested, and found not to hold. We comment on properties that the solution must have in an unsuccessful attempt to find an alternative conjecture. In addition we obtain estimates for the location of various non-physical singularities.

The remainder of the paper is organized as follows. In section 2 we briefly describe the finite-lattice method of series expansions, give details regarding the specific implementations for the Kagomé and honeycomb lattices, and show how the finite-lattice method can be supplemented by an extension procedure allowing us to derive more series terms. Details regarding the analysis of the series are given in section 3 and the implications for possible conjectures for the critical point on the Kagomé lattice are discussed in section 4. A brief summary and discussion is given in section 5.

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2. Series expansions

The q-states Potts model is defined on a lattice in terms of a 'spin' variable, σ_j on each site j, with integer values from 0 to $q-1$. With the use of the δ-function, $\delta(x, y) = 1$ if $x = y$ and 0 otherwise, the Hamiltonian describing the Potts model in a homogeneous magnetic field h can be written

$$\mathcal{H} = J \sum_{\langle ij \rangle} (1 - \delta(\sigma_i, \sigma_j)) + h \sum_i (1 - \delta(\sigma_i, 0)) \tag{1}$$

where the first sum is over interacting pairs and the second over sites. The constants are chosen so that the ground state ($\sigma_i = 0 \forall i$) has zero energy. In this work we shall only consider the case in which the spin–spin interactions are restricted to nearest-neighbour sites.

The low-temperature expansion is based on perturbations from the fully aligned ground state and is expressed in terms of the low-temperature variable $u = \exp(-J/k_B T)$ and the field variable $\mu = \exp(-h/k_B T)$. The expansion of the partition function in powers of u may be expressed as

$$Z = \sum_{n=0}^{\infty} u^n \Psi_n(\mu) \tag{2}$$

where $\Psi_n(\mu)$ are polynomials in μ. It is more convenient to express the field dependence in terms of the variable $x = 1 - \mu$ and truncate the expansion at x^2

$$Z = Z_0(u) + x Z_1(u) + x^2 Z_2(u) + \cdots$$

where $Z_n(u)$ is a series in u formed by collecting all terms in the expansion of Z containing factors of x^n. Standard definitions yield the magnetization

$$M(u) = M(0) + \frac{q}{q-1} Z_1(u)/Z_0(u) \tag{3}$$

the zero-field susceptibility

$$\chi(u) = 2\frac{Z_2(u)}{Z_0(u)} - \frac{Z_1(u)}{Z_0(u)} - \left(\frac{Z_1(u)}{Z_0(u)}\right)^2 \tag{4}$$

and the specific heat

$$C_v(u) = (\beta J)^2 \left(u \frac{\mathrm{d}}{\mathrm{d}u}\right)^2 \ln Z_0(u). \tag{5}$$

So in order to obtain the series expansions of the specific heat, spontaneous magnetization and the susceptibility it suffices to calculate the three quantities Z_0, Z_1 and Z_2.

2.1. The finite-lattice method

We refer to the recent review [8] by Enting for background material and references regarding the existence of series expansions as well as the foundations and many applications of the finite-lattice method. On the square lattice the infinite-lattice partition function Z can be approximated by a product of partition functions $Z_{m,n}$ on *finite* $(m \times n)$ lattices,

$$Z(u) \approx \prod_{m,n} Z_{m,n}(u)^{a_{m,n}} \qquad \text{with } m + n \leqslant r \tag{6}$$

where r is a cut-off which limits the size of the rectangles considered. For the low-temperature expansion of the Potts model $Z_{m,n}$ is calculated by summing the Boltzmann

weights over all spin configurations on the finite lattice. All spins outside the $m \times n$ rectangle are fixed at 0. The weights $a_{m,n}$ are known explicitly [9],

$$a_{m,n} = \begin{cases} 1 & \text{for } n+m = r \\ -3 & \text{for } n+m = r-1 \\ 3 & \text{for } n+m = r-2 \\ -1 & \text{for } n+m = r-3 \\ 0 & \text{otherwise.} \end{cases} \tag{7}$$

Rectangles are obviously the natural finite-lattice building blocks on the square lattice. However, since the weights $a_{m,n}$ depend only on the topology of the finite lattices, one can actually use rectangles as the finite-lattice blocks on any two-dimensional lattice. One merely has to use a more complicated unit cell in building the rectangles. Due to the symmetry of the lattices one generally has $Z_{m,n} = Z_{n,m}$ so one need only consider the case $m \leqslant n$ and change the weights $a_{m,n}$ correspondingly, i.e. multiply by two if $m < n$. The number of terms derived correctly with the finite lattice method is given by the power of the lowest-order connected graph not contained in any of the rectangles considered, which in this case are chains of sites all in the same state ($\neq 0$). From the Potts Hamiltonian we see that on a lattice where each site has m neighbours, chains of length s give rise to terms of order $N_r = (m-2)r + 2$ in u. For a given value r (the semi-perimeter of the largest rectangle) the series expansion is thus correct to an order N_r determined by the length of the smallest chain that does not fit into any of the rectangles. So in a calculation of $Z_{m,n}(u)$ one can safely truncate the polynomials just above N_r.

2.2. The transfer-matrix technique

The efficient way of calculating $Z_{m,n}$ is by transfer-matrix techniques. From the Potts Hamiltonian (1) we see that the evaluation of $Z_{m,n}$ only involves contributions from interactions between nearest-neighbour spins and interactions between the spins and the magnetic field. The sum over all configurations can therefore be performed by moving a *boundary* line through the lattice. At any given stage the boundary cuts through a number of, say k, sites. In the q-state Potts model there are a total of q^k different configurations along the boundary. We shall refer to each such specific configuration as a 'signature'. For each signature we construct a partial sum which is the Boltzmann weight associated with all possible states on the part of the lattice already traversed by the boundary. Each partial sum is a (truncated) polynomial in u. The most efficient way to move the boundary is by adding one 'cell' at a time. Shifting the boundary corresponds to generating a new vector of q^k partial sums from a previous vector. Formally this is a matrix operation. In practice, it is possible to avoid explicit use of the transfer matrix due to the move being local. Nevertheless, we will continue to use the term 'transfer-matrix technique' for this type of transformation of vectors of partial sums. Evaluating $Z_{m,n}$ involves $m \times n$ iterations of q^m series operations. In terms of the cut-off r used in equation (6), the main growth in both memory and time requirements comes from a factor $q^{r/2}$. Since the Potts Hamiltonian only singles out the '0' state, the remaining $q-1$ states are equivalent, i.e. any permutation among the non-zero states in a signature will leave the associated polynomial unchanged. For example, one may interchange the states '1' and '2' without changing the Boltzmann weight of the configurations. This effectively means that the number of different signatures one needs to store can be reduced by a factor of $(q-1)!$, since one need only keep one specific representative signature for each equivalence class. However, due to the

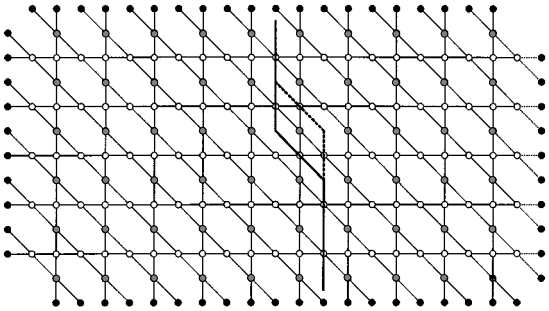

Figure 1. A snapshot of the boundary (heavy full line) during the transfer-matrix calculation on the Kagomé lattice. Full circles indicate the spins in the ground state bounding the rectangle, shaded circles indicate 'shadow' sites, while open circles are the sites cut by the boundary line at some point during the calculation.

implementation of the algorithms utilizing this reduction is only useful for $q \geqslant 4$, since the use of equivalence classes of signatures doubles the memory requirements. In short the total memory requirement for the q-state Potts model grows like $2q^{r/2}/(q-1)!$.

The calculation of the series expansion involve only additions and multiplications, so in order to deal with the large integer coefficients occurring in the series expansions the calculations should be performed using modular arithmetic [10]. This involves performing the calculation modulo of various prime numbers p_i and then reconstructing the full integer coefficients at the end. The Chinese remainder theorem ensures that any integer has a unique representation in terms of residues. If the largest absolute values occurring in the final expansion is M then we have to use a number of primes n so that $p_1 p_2 \ldots p_n/2 > M$. Note that it is not necessary to be able to uniquely reproduce the intermediate values, which can be much larger than the final ones.

2.2.1. Kagomé lattice specifics. Figure 1 shows a snapshot of the boundary (the heavy full line) during the traversing of the lattice. The Boltzmann weights of spin–spin and field–spin interactions on sites to the left of the boundary line have already been included in the partial sums. The part of the lattice to the right of the boundary is to be included subsequently. In order to add a new 'cell' to the completed part of the lattice, the boundary is moved to a new position as indicated by the heavy dotted line. The partial sums have to be updated in order to pick up the Boltzmann weights from the six spin–spin interactions between the five sites lying between the old and new positions of the boundary line. In addition the Boltzmann weights from the field interacting with the 'shadow' spin at the centre (shaded) site and the two sites cutting the dotted line has to be included. We use the term 'shadow' spin to denote spins placed on sites of the underlying lattice which are never cut by the boundary line (or belong to the border) and therefore do not have to be stored in a signature. Note that in this updating the weights do not depend on the states of any sites on the boundary line other than the two sites involved in the move. Let S_{σ_b,σ_t} denote a boundary which has the spins on the bottom and top sites of the moving section of the boundary in state σ_b and σ_t, respectively. The partial sum after the move to the new position $W(S_{\sigma_b',\sigma_t'}, u, x)$, is obtained by summing over the q^2 partial sums $W(S_{\sigma_b,\sigma_t}, u, x)$, multiplied by the appropriate Boltzmann weights

$$W(S_{\sigma_b',\sigma_t'}, u, x) = B_h(\sigma_b')B_h(\sigma_t') \sum_{\sigma_b,\sigma_t} B_W(\sigma_b, \sigma_t, \sigma_b', \sigma_t')W(S_{\sigma_b,\sigma_t}, u, x) \qquad (8)$$

where the weight B_W is obtained by summing over the q-states σ_c of the centre spin at the site indicated by a shaded circle between the two positions of the boundary line

$$B_W(\sigma_b, \sigma_t, \sigma_b', \sigma_t') = \sum_{\sigma_c} B_h(\sigma_c) B_T(\sigma_b, \sigma_b') B_T(\sigma_t, \sigma_t') B_T(\sigma_b, \sigma_c) \times B_T(\sigma_b', \sigma_c) B_T(\sigma_t, \sigma_c) B_T(\sigma_t', \sigma_c) \tag{9}$$

and the 'elementary' Boltzmann weights are

$$B_T(\sigma_i, \sigma_j) = u^{1-\delta(\sigma_i,\sigma_j)} \qquad B_h(\sigma_i) = (1-x)^{1-\delta(\sigma_i,0)}. \tag{10}$$

The updating at the bottom and top boundaries is of course slightly different since only a single site has to be moved. The weights involved are easily deduced from the general case above. The initial weight assigned to a given signature S, when the boundary line is all the way to the left in figure 1, is simply $((1-x)u^2)^{k_S}$, where k_S is the number of non-zero states in S. The value $Z_{m,n}$ is calculated after the boundary has been moved n columns to the right and is positioned at the right border in figure 1. At this point only the interactions (indicated by the dotted lines) between the 'internal' spins along the boundary and the spins just outside the rectangle (which are all in the ground state) have to be added, hence $Z_{m,n}(u,x) = \sum_S u^{2k_S} W(S,u,x)$. Since we need not change the weight $W(S,u,x)$ of the signature S we can proceed and add the next column of sites in order to calculate $Z_{m,n+1}$. In this way one builds up the finite lattices of width m one column at a time with each column built up one cell at a time. The cut-off $r_{\max}$ in the length of the perimeter of the finite lattices is obviously determined by the largest width, $w_{\max}$ that the available memory allows us to represent, $r_{\max} = 2w_{\max} + 1$.

2.2.2. Honeycomb lattice specifics. Figure 2 shows a snapshot of the boundary (the heavy full line) during the calculation. In this case only a single site at a position k on the boundary line is moved (as indicated by the heavy dotted line) in order to add a new 'cell' to the completed part of the lattice. Note that in this updating the weights also depend on the state of the site immediately below the site involved in the actual move. The partial sum after the move to the new position, $W(S_{\sigma_k'}, u, x)$, is obtained much as before by summing over the partial sums $W(S_{\sigma_k}, u, x)$

$$W(S_{\sigma_k'}, u, x) = B_h(\sigma_k') \sum_{\sigma_k} B_W(\sigma_k, \sigma_k') W(S_{\sigma_k}, u, x) \tag{11}$$

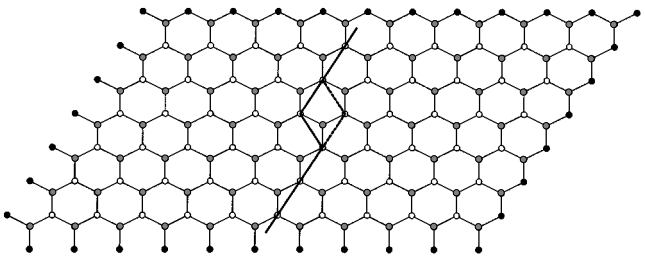

Figure 2. A snapshot of the boundary (heavy full line) during the transfer-matrix calculation on the honeycomb lattice. Full circles indicate the spins in the ground state bounding the rectangle, shaded circles indicate 'shadow' sites, while open circles are the sites cut by the boundary line at some point during the calculation.

where B_W is

$$B_W(\sigma_k, \sigma_k') = \sum_{\sigma_c} B_h(\sigma_c) B_T(\sigma_k', \sigma_c) B_T(\sigma_k, \sigma_c) B_T(\sigma_{k-1}, \sigma_c). \tag{12}$$

Again the updating on the top and bottom borders are a little different. This time the initial weight of a signature is 0 apart from the all-zero signature which has weight 1. This corresponds to the boundary line initially being positioned to the left on the spins fixed in the ground state. The finite-lattice partition function $Z_{m,n}$ is simply the weight of the all-zero signature after $n+1$ moves to the right.

2.3. Extension procedure

In a recent paper [11] it was shown how the finite-lattice method, applied to low-temperature series for the spin-1 Ising model on the square lattice, can be supplemented by an extension procedure allowing one to derive more series terms correctly. As already noted the finite-lattice calculations result in a series correct to an order N_r growing linearly with r. The first incorrect term is due to the smallest connected graphs, e.g. a linear chain of sites, not contained in any of the rectangles with a perimeter smaller than r. However, there are typically only a few such graphs and the vast majority of graphs contributing to orders just above N_r have been counted. The series for $Z_n(u)$ can be extended by looking at 'correction terms' to the finite lattice contributions. For each $r \leqslant r_{\max}$ and $n \leqslant 2$ we calculate the truncated polynomials $Z_{n,r} = \sum_j z_{n,r,j} u^j$ correct to order $N_r + 15$. Then we look at the integer sequences $d_{n,s}(r)$ obtained by taking the difference between successive polynomials

$$Z_{n,r+1}(u) - Z_{n,r}(u) = u^{N_r+1} \sum_{s \geqslant 0} (z_{n,r+1,N_r+s+1} - z_{n,r,N_r+s+1}) u^s = u^{N_r+1} \sum_{s \geqslant 0} d_{n,s}(r) u^s. \tag{13}$$

The first of these correction terms $d_{n,0}(r)$ is often a simple sequence which one can readily identify. Once this correction term is identified as a function of r one can use it to obtain an extra term in the series expansion of $Z_n(u)$ from the term of order $N_{r_{\max}} + 1$ in $Z_{n,r_{\max}}$. Similarly one can obtain further series terms if one can find formulae for the higher-order correction terms $d_{n,s}(r)$.

2.3.1. Kagomé lattice. For $q = 3$ we find that the sequence $d_{0,0}(r)$ starts as

$$16, 8, 72, 144, 288, 576, 1152, 2304, 4608, 9216, 18\,432, \ldots$$

from which it is immediately clear that $d_{0,0}(r) = 9 \times 2^r$ for $r \geqslant 3$. Similarly we find that the next sequence $d_{0,1}(r)$ start as

$$12, 48, 132, 336, 816, 1920, 4416, 9984, 22\,272, 49\,152, 107\,520, \ldots$$

and we see find that $d_{0,1}(r) = (9r + 6)2^{r-1}$ for $r \geqslant 3$. And indeed we find that $d_{n,s}(r)/2^r$ is expressible as a polynomial in r with the general formula given by

$$d_{n,s}(r)/2^r = \sum_{k=0}^{s+n} a_{s,k} r^k + \mathrm{mod}(r, 2) \sum_{k=0}^{\lfloor r/2 \rfloor - 1 + n} b_{s,k} r^k \qquad \text{for } r \geqslant \max(3, s+2). \tag{14}$$

These general expressions for the correction terms are also valid for the $q = 4$ case. For $q = 3$ we used the integer sequences for $d_{n,s}(r)$, known from the finite-lattice calculation up to $r_{\max} - 1 = 26$ to find formulae for all correction terms up to $s = 9$ for Z_0 and Z_1, and up to $s = 8$ for Z_2. For $q = 4$, where the sequences are known up to $r_{\max} - 1 = 22$, we found the formulae for the correction terms up to $s = 8$, 7, and 6 for Z_0, Z_1, and Z_2,

respectively. This in turn allowed us to calculate the series for the specific heat, spontaneous magnetization, and zero-field susceptibility, correct to order 67, 67, and 66 for $q = 3$, and 58, 57, and 56 for $q = 4$. The resulting series are listed in tables 1 and 2.

2.3.2. Honeycomb lattice. The extension procedure for the 3-state Potts model on the honeycomb lattice is essentially the same as for the Kagomé lattice. The major difference is that rather than looking at the difference between successive expansions of Z_n for each perimeter length r, we look at each width w and thus perimeter lengths $r = 2w + 1$. For a given width the expansion is correct to order $2w + 2$. In this case the correction terms are simply given by polynomials of order $2s + n$. We managed to find the formulae for the first five correction terms for Z_0, and Z_1 and the first four for Z_2. This enabled us to calculate the series for the specific heat and magnetization to order 35 while the susceptibility was calculated to order 34. The resulting series are listed in table 3.

3. Analysis of the series

The series were analysed using differential approximants (see [12] for a comprehensive review), which allows us to locate the singularities and estimate the associated critical exponents fairly accurately, even in cases where there are many singularities. Here it suffices to say that a Kth-order differential approximant to a function f, for which one has derived a series expansion, is formed by matching the coefficients in the polynomials Q_i and P of order N_i and L, respective, so that the solution to the inhomogeneous differential equation

$$\sum_{i=0}^{K} Q_i(x) \left(x \frac{\mathrm{d}}{\mathrm{d}x} \right)^i \tilde{f}(x) = P(x) \tag{15}$$

agrees with the first series coefficients of f. The equations are readily solved as long as the total number of unknown coefficients in the polynomials is smaller than the order of the series N. The possible singularities of the series appear as the zeros x_i of the polynomial Q_K and the associated critical exponent λ_i is estimated from the indicial equation

$$\lambda_i = K - 1 - \frac{Q_{K-1}(x_i)}{x_i Q'_K(x_i)}.$$

Since the critical exponents of the Potts model are known exactly, one may use these to obtain improved estimates for the critical point u_c. A simple method consists of generating a large number of estimates for u_c and the associated critical exponent from a variety of high-order differential approximants and then performing a (linear) fit on the data set $(u_c, \lambda - \lambda_c)$, where λ is the known exponent and λ_c the estimate from a given approximant. In this way the 'true' critical point is given by the intersection with the ordinate axis.

In order to locate the non-physical singularities of the series in a systematic fashion we used the following procedure: we calculated all first- and second-order inhomogeneous differential approximants with $|N_i - N_j| \leqslant 1$ and $L \leqslant 10$, which use more than $N - 10$ terms for the Kagomé series and $N - 6$ terms for the honeycomb series, respectively. Each approximant yields N_K possible singularities and associated exponents from the N_K zeros of Q_1 or Q_2, respectively (many of these are of course not actual singularities of the series but merely spurious zeros.) Next these zeros are sorted into equivalence classes by the criterion that they lie at most a distance 2^{-k} apart. An equivalence class is accepted as a singularity if it contains more than 75% of all approximants, and an estimate for the singularity and exponent is obtained by averaging over the approximants (the spread among

Table 1. Low-temperature series for the 3-state Kagomé lattice Potts model magnetization ($M(u) = \sum_n m_n u^n$), susceptibility ($\chi(u) = \sum_n x_n u^n$), and specific heat ($C_v(u) = \sum_n c_n u^n$).

n	m_n	x_n	c_n
0	1	0	0
1	0	0	0
2	0	0	0
3	0	0	0
4	−3	6	96
5	0	0	0
6	−18	84	576
7	−12	48	588
8	−87	738	2304
9	−120	816	5832
10	−432	5520	10800
11	−840	8904	36300
12	−2883	49662	84960
13	−5208	79200	198744
14	−21378	449028	750288
15	−39876	812352	1500300
16	−144507	3772350	5268480
17	−309456	7762032	12588840
18	−978888	31487916	35120088
19	−2349828	72083112	98916888
20	−6995931	266083134	260218080
21	−17727576	654302352	750052800
22	−52099902	2277479412	2076871104
23	−133195908	5812957368	5659178520
24	−389599548	19418064216	16308196992
25	−1010029956	51144852552	43665390000
26	−2921670744	165263023776	125610109872
27	−7740553548	447259989384	344058507576
28	−22113581814	1406988933456	973947846816
29	−59567197308	3884885652408	2717471043624
30	−168833343960	11978733643956	7640481476880
31	−459072147672	33528134442816	21375599418720
32	−1297493365242	101944430318280	60315824916480
33	−3550587103272	288136319393496	168526829468052
34	−10020565843764	866916682806576	477304061147760
35	−27578939587200	2468399305985472	1336067341489440
36	−77700379317777	7364816760006162	3783098028982752
37	−214929171165696	21086188343928000	10627245862050204
38	−604752691194156	62508036269127720	30055832138045448
39	−1679515789816584	179683432691259264	84661883836108488
40	−4723546882412469	530069803229979774	239473055786181120
41	−13158053809070472	1528013328153162432	675545581702034388
42	−37007705334935184	4490951557780006500	1912468636319315760
43	−103340887711777872	12971616570246628752	5400539890817982372
44	−290710029319950927	38013955581535924626	15298868946943164000
45	−813474856495634532	109953447580362728424	43250175040705306560
46	−2289096438867426030	321487932175448055060	122570584529158036272
47	−6416856975936308364	930787060871870632176	346895918095745946468
48	−18064395265699321722	2716589975688019383024	983504007524475320832
49	−50714600486264652300	787016592758494947271 2	278604150363940460 4300
50	−142840830525954114798	229370366510582344054 20	790270060068805277 4000
51	−401528506770385674492	664760993073975491698 32	224031312272015682877 44
52	−113154666306655147842	193517645617988549126424	635789330468699826831 36
53	−318434908272205811851 2	560973640191718094985096	180357253144546436992860
54	−897882126761020681426 2	163151779530431684157218 4	512082087271230348883152
55	−252927497929505754474 60	472991618863264225192418 4	145353790630955675269050 0
56	−713572147062179295799 62	137457621169249515418107 00	412875888758834993646873 6
57	−201185127578571697041 084	398502598984282620496602 48	117259474994135913067655 40
58	−567909244934815644951 876	115736001230869629237320 376	333212129397269432081002 08
59	−160242874837359420078 3516	335508831559907827237662 504	946817199409033145381998 08
60	−452583072151490945252 0484	973882929999796303949590 356	269161157458651526754760 800
61	−127793134529985625757 51088	282290656035119245672662 8808	765164597112272168946822 924
62	−361124130228321697578 63636	819028096442150166818062 4496	217603557444582418070570 1792
63	−102034772613523534358 123196	237372388837401177193188 76968	618856672226006122569581 7348
64	−288481688315871423868 448841	688428558531508184039365 15902	176058425274159844033259 52000
65	−815585466811800742541 072412	199491232724918682054607 418184	500897739290363773082079 13920
66	−230702236179765869934 9383748	578362795330018152263654 517708	142548622063270027563999 134952
67	−652593564028043157154 6633332		405705851976987914121136 482468

Table 2. Low-temperature series for the 4-state Kagomé lattice Potts model magnetization ($M(u) = \sum_n m_n u^n$), susceptibility ($\chi(u) = \sum_n x_n u^n$), and specific heat ($C_v(u) = \sum_n c_n u^n$).

n	m_n	x_n	c_n
0	1	0	0
1	0	0	0
2	0	0	0
3	0	0	0
4	−4	9	144
5	0	0	0
6	−24	126	864
7	−32	144	1764
8	−120	1179	3168
9	−336	2556	18468
10	−768	10332	25200
11	−2496	29952	117612
12	−6612	109053	301104
13	−17296	293580	736164
14	−61176	1221390	3083472
15	−150016	3269736	7009200
16	−518308	12652155	26587584
17	−1418576	36719028	75949200
18	−4266064	126768168	220443768
19	−12800864	392732064	728295840
20	−36773692	1284178329	1994796720
21	−112996720	4104726084	6533132760
22	−334128168	13312704402	19485485712
23	−1009728992	42563828232	59845160592
24	−3068945888	138178786131	189326190240
25	−9160795472	439049042172	566841960000
26	−27959064832	1420005679128	1785253830984
27	−83967142416	4516071938172	5433825702492
28	−255193684244	14525756839035	16774055209296
29	−775172669984	46381825905912	52134557758884
30	−2353166401072	148568699237004	160066296276120
31	−7183969493024	474997804689384	499465339589736
32	−21865038292880	1518337263464217	1542088839821184
33	−66761010187600	4848910682677956	4785625241692812
34	−203920895329384	15488026787092734	14861921154785280
35	−622939137585200	49405076991181620	46013136930629820
36	−1907597954601412	157717547673256251	143179724710028592
37	−5839100589367264	502842226178206728	444307460788537128
38	−17904553293987416	1603882835785276794	1382007017890018224
39	−54924288884555312	5111833437525631932	4299991262500266216
40	−168587657364598336	16290829522698292881	13372271008660815840
41	−517972188102818880	51898455026560227384	41650080676866915192
42	−1591935301954375608	165292258036343046786	129636781648513933248
43	−4896801346851222432	526315378561652140848	403873766750144048472
44	−15070594422813138572	167552563168545625689 3	125856411675555553322 72
45	−46407033247825344416	533261594752895510884 8	392250625328985827454 0
46	−142993519851275783136	1696934600330689089259 2	122331216816710154812 88
47	−440788726279046174896	5398534303690895541262 8	381510826262908443227 52
48	−1359532990978694337372	1717205200011649482786 81	119034204865510152257 856
49	−4195096334194601911072	5461047379216091448558 00	371474973016958736250 164
50	−12950662558102405142952	1736438666544106710588 234	115951395777348251397 6000
51	−39998406500348447841296	5520377782897940654049 924	362050429371037115642 1864
52	−12358554697535175462 9604	1754722587972923239446 4257	113065252039446642794 53296
53	−38201211234223789456 9232	5576756391616327339597 7652	353192189589395923218 18012
54	−11812816057886575035 58720	1772111084670023258231 32392	110351918838492476547 124032
55	−36542027068968334842 75232	5630374801524447724312 78776	344852285944713292340 450460
56	−11308157611732259902 019808	1788651804062931187123 534599	107790940856029191832 6803360
57	−35005816685168912890 325088		336979786965084685892 2769964
58			105368779857386557489 62377952

Table 3. Low-temperature series for the 3-state honeycomb lattice Potts model magnetization ($M(u) = \sum_n m_n u^n$), susceptibility ($\chi(u) = \sum_n x_n u^n$), and specific heat ($C_v(u) = \sum_n c_n u^n$).

n	m_n	x_n	c_n
0	1	0	0
1	0	0	0
2	0	0	0
3	−3	4	36
4	−9	24	96
5	−36	132	450
6	−123	672	1368
7	−450	3192	5292
8	−1764	15996	20352
9	−6690	74396	79650
10	−26649	354936	324000
11	−104112	1639764	1285020
12	−421248	7669876	5346720
13	−1688337	35282064	21788832
14	−6888978	162809928	91199976
15	−28063296	745459776	378084780
16	−115459524	3413032716	1590491136
17	−475617330	15560103924	6669799788
18	−1970737233	70861321612	28184656536
19	−8184006855	321879751956	119093015550
20	−34118533647	1460223461700	505409136480
21	−142565353488	6612700085376	2147032241928
22	−597406140090	29909912167920	9145594625376
23	−2508667475949	135106788553176	39007441263438
24	−10558028568744	609650115022656	166688869662720
25	−44517381753474	2748066368017884	713206171161000
26	−188048310460236	12375977640193200	3055980598701576
27	−795629660236428	55687114737623036	13109375226995928
28	−3371492077402095	250375275986449380	56301379329483456
29	−14306836317209163	1124888495649710904	242042552346534858
30	−60791276536672623	5050512588212291864	1041567142751412840
31	−258626141584492419	22661449251743675976	4486041205757057268
32	−1101554410568672223	101621602207472708064	19337534732644964352
33	−4696874651300269557	455455915765485083232	83420329126988297664
34	−20047233485072891340	2040254076696411350796	360128233701907804440
35	−85647742067290024089		1555734167361870299160

the approximants is also calculated.) The calculation was then repeated for $k-1, k-2, \ldots,$ until a minimal value of 5. To avoid outputting well converged singularities at every level, once an equivalence class has been accepted, the approximants which are members of it are removed, and the subsequent analysis is carried out on the remaining data only. One advantage of this method is that spurious outliers, a few of which will almost always be present when so many approximants are generated, are discarded systematically and automatically.

3.1. Kagomé lattice results

In figure 3 we have plotted the estimates of the critical exponents versus the estimates for the critical point for the 3-states Potts model on the Kagomé lattice. The data was obtained

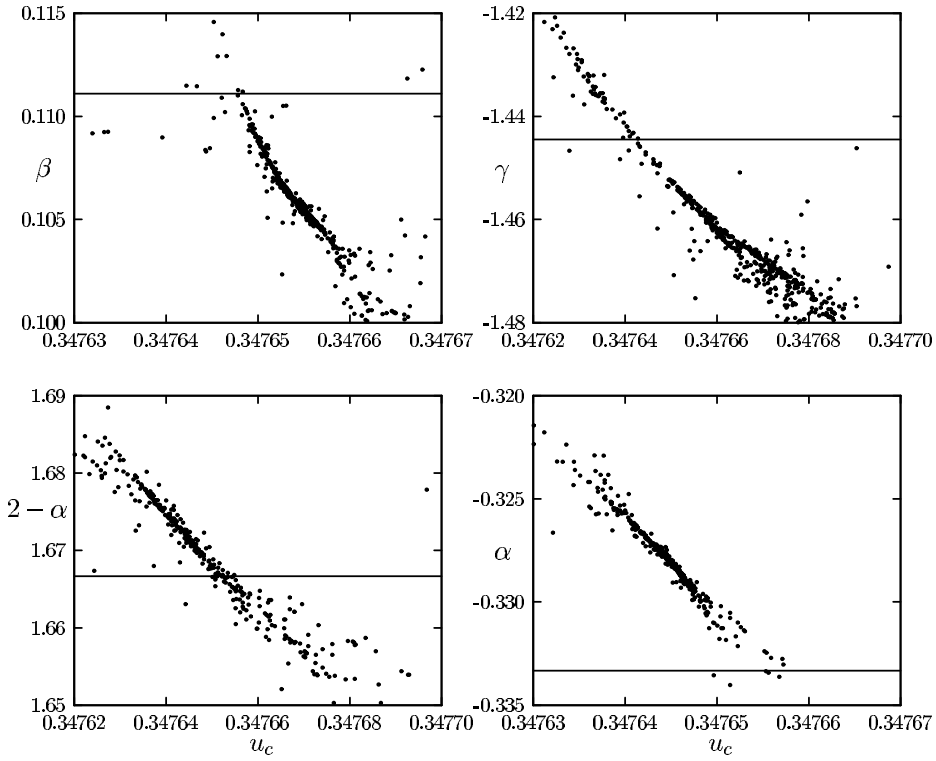

Figure 3. Plots of the estimates of the critical exponents β, γ, $2-\alpha$, and α, respectively, versus the critical point u_c, as obtained from first- and second-order differential approximants to the series for the magnetization (top left), susceptibility (top right), partition function (bottom left), and specific heat (bottom right) for the 3-state Potts model on the Kagomé lattice. The full lines indicate the exact values of the exponents.

from first- and second-order inhomogeneous differential approximants to the series for the spontaneous magnetization, susceptibility, zero-field partition function Z_0, and specific heat. In the case of the susceptibility and specific heat we analysed the series $\chi(u)/u^4$ and $C_v(u)/u^4$. The data includes the results from approximants with $L \leqslant 10$, $|N_i - N_j| \leqslant 1$ and where at least 55 series terms were used in the case of $M(u)$ and $Z_0(u)$, while at least 50 terms were used in the case of $\chi(u)/u^4$ and $C_v(u)/u^4$. From the intersect between the data points and the lines indicating the exact critical exponents we estimate that $u_c = 0.347\,648(10)$, where the number(s) in parentheses indicate our estimate for the error in the last digit(s).

Figure 4 shows the estimates of the critical exponents versus the estimates for the critical point for the 4-states model. In this case the data includes the results from approximants using at least 45 of the series terms for $M(u)$ and $Z_0(u)$ and 40 terms for $\chi(u)/u^4$ and $C_v(u)/u^4$. In this case there is a quite large discrepancy between the u_c estimates obtained from the four series. The partition function and specific heat yields estimates around $u_c = 0.317\,25(15)$, while no reasonable extrapolation is possible from the susceptibility series. However, for all these series the exponent estimates are generally quite far from the exact results. Only the magnetization series yields exponent estimates close to the known value, and based on this series we estimate $u_c = 0.316\,85(5)$.

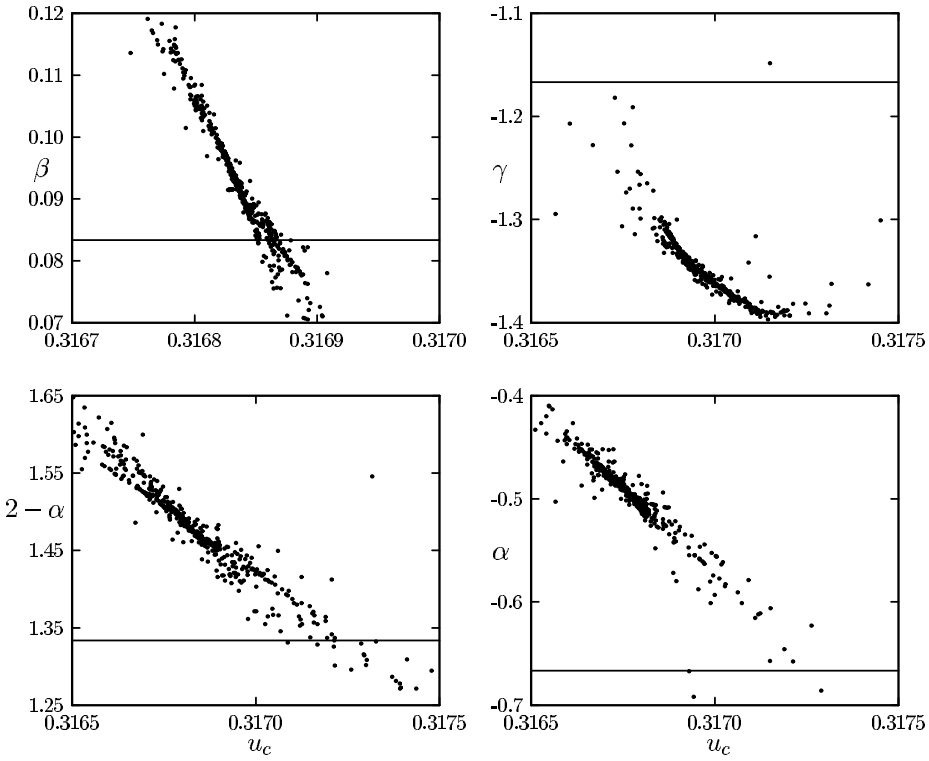

Figure 4. Same as in figure 3, but for the 4-state model.

3.2. Honeycomb lattice results

For the honeycomb lattice the critical point is determined by the positive real root (closest to the origin) of the equation [7]

$$w^3 - 3w - \sqrt{q} = 0 \tag{16}$$

where $w = (\exp[J/k_BT] - 1)/\sqrt{q}$. The fully anisotropic version of this result is given in [13]. This result is known to be correct for $q \geqslant 4$ and $q = 2$, but for $q = 3$ it relies on the existence of a single phase transition. Given this entirely likely situation, duality arguments give the critical point. Setting $q = 3$ in this equation leads to the critical point, $u_c = 0.226\,6815\ldots$, the validity of which is confirmed by our series analysis presented below. As before we have chosen to plot, in figure 5, exponent estimates versus the estimates for the critical point. In this case the data includes approximants using at least 25 of the series terms for $M(u)$ and $Z_0(u)$ and 20 terms for $\chi(u)/u^3$ and $C_v(u)/u^3$. The series for the magnetization and partition function yield estimates very close to the intersection between the exact critical exponent and the exact u_c. Though the remaining series, in particular the susceptibility, deviate further from the expected intersection the resulting estimates for the critical point lie on either side of the exact value. It is thus clear from this series analysis that the results are fully consistent with the exact value for the critical point.

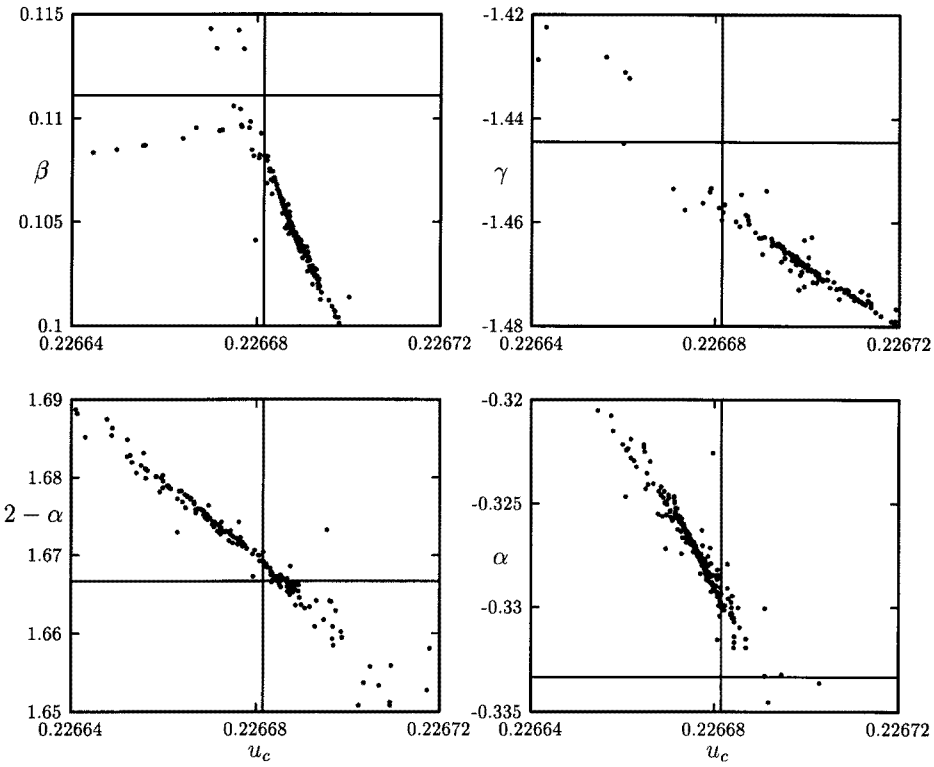

Figure 5. Same as in figure 3, but for the 3-state Potts model on the honeycomb lattice. The full lines indicate the exact values of the exponents (horizontal) and u_c (vertical).

3.3. Analysis of non-physical singularities

As well as the physical singularities, the other singularities in the complex plane are also of interest, as discussed in the case of the square-lattice Potts model by Matveev and Shrock [14]. However, while the location of such singularities can be reasonably accurately estimated from the differential approximants to the series, we have found the exponent estimates to be much more problematic. To illustrate this, we note that in 1994 we [15] extended the spin-1 square lattice low-temperature series to 79 terms, and found non-physical singularities in the magnetization series at $u_- = -0.598\,53(4)$ with exponent $\beta_- = 0.1247(6)$ and a pair of complex singularities at $u_\pm = -0.301\,83(5) \pm 0.378\,70\mathrm{i}$ with exponent $\beta_\pm = -0.127(3)$. In 1996 we [11] were able to further extend the series to 113 terms, and a reanalysis led to the exponent estimates $\beta_\pm = -0.1690(2)$. In particular, we note that even for the physical singularity, the dlog Padé approximants are seemingly well converged, and an exponent estimate based only on the central value and two standard deviations would give a confidence limit that excluded the correct result. In the light of the above comments, we give estimates of the critical exponents for the non-physical singularities, but without quoting confidence limits, as we do not believe we can do so in any meaningful way. Consequently, the exponent estimates should be viewed as 'indicative' or a 'best guess'.

For the 3-state honeycomb lattice Potts model, we find a non-physical singularity on the negative real axis at $u_- = -0.363(3)$ with *apparent* exponents $\alpha_- = 0.5$, $\beta_- = 0.11$,

and $\gamma_- = 1.15$, but as we argue below, we don't believe these estimates. We find a further complex-conjugate pair of singularities at $u_\pm = -0.06(2) \pm 0.47(3)\mathrm{i}$ with a weakly *divergent* magnetization, and specific heat and susceptibility exponents around one. The singularity on the negative real axis is the duality mapping (see e.g. [2]) of the triangular-lattice anti-ferromagnetic critical point, via the relation $\mathrm{e}^{K_H} = 1 - q/(1 - \mathrm{e}^{-K_\mathrm{c}})$. The singularity $\mathrm{e}^{-K_H} = -0.363$ then maps to $\mathrm{e}^{K_T} = 0.201(2)$, which agrees with the earlier study of the Potts triangular-lattice anti-ferromagnet [16] in which the estimate $\mathrm{e}^{K_T} = 0.204(3)$ was obtained. However, it is known that the Potts anti-ferromagnetic on the triangular lattice has a weak first-order transition [17–19] and an ordered ground state. Thus the exponents we observed are spurious, and follow from an implicit assumption of a second-order transition. A very interesting approach to the honeycomb q-state Potts model has recently been made by Maillard [20], in an attempt to utilize the symmetries of models for which there is no Yang–Baxter structure. For values of q equal to the Tutte–Beraha numbers, infinite-order groups become of finite order. For such values of q one still gets groups which grow exponentially, except for the cases $q = 1, 3$. Utilizing this observation, Maillard systematically constructs invariants which are expected to be appropriate for the 3-state model on the honeycomb lattice. From these invariants, one expects singularities to occur at some or all of the zeros of $u^3 - 3u - 1 = 0$, which gives as one zero $u = -0.347\,29\ldots$, which is some 4% away from the observed position of the singularity on the negative real axis. As our confidence limit on the position of the singularity in question is better than 1%, it is unlikely—but not impossible—that the Maillard prediction is correct for this singularity.

For the 3-state Kagomé-lattice Potts model, we find a non-physical singularity on the negative real axis at $u_- = -0.4023(5)$ with exponents indistinguishable from the exponents at the physical singularity. We also find four conjugate pairs of singularities at $u_{\pm 1} = 0.38(2) \pm 0.24(2)\mathrm{i}$, $u_{\pm 2} = 0.278(10) \pm 0.38(1)\mathrm{i}$, $u_{\pm 3} = -0.113(6) \pm 0.515(10)\mathrm{i}$, and $u_{\pm 4} = -0.37(2) \pm 0.30(5)\mathrm{i}$. At $u_{\pm 1}$ there appears to be a divergent magnetization and susceptibility, but a non-divergent specific heat. At $u_{\pm 2}$ and $u_{\pm 4}$ all three thermodynamic quantities appear to be divergent, while at $u_{\pm 3}$ there appears to be a divergent specific heat and susceptibility, but a non-divergent magnetization.

For the 4-state Kagomé-lattice Potts model, we find a non-physical singularity on the negative real axis at $u_- = -0.42(1)$ with exponents we cannot estimate. We also find two conjugate pairs of singularities at $u_{\pm 1} = 0.275(10) \pm 0.305(10)\mathrm{i}$, and $u_{\pm 2} = -0.345(10) \pm 0.235(1)\mathrm{i}$. At both $u_{\pm 1}$ and $u_{\pm 2}$ all three thermodynamic quantities appear to be divergent. While we are confident that these non-physical singularities are accurately estimated from our analysis, we note that there are probably some additional singularities which we have not been able to find. In particular we expect that the number of non-physical singularities grows with q, as is the case for the spin-S Ising model [21].

4. Critical point of the q-state Potts model on the Kagomé lattice

Unlike the square, triangular and honeycomb lattice, the critical point of the q-state Potts model on the Kagomé lattice is not known. For some values of q, notably $q = 0$ and $q = 2$ it is known, and some years ago Wu [3] conjectured the result for general q, while Tsallis [22] made a different conjecture. The Wu conjecture is known not to hold for $q = 3$ [16], as it leads to an incorrect phase boundary. Both conjectures agree for the (known) case $q = 2$, corresponding to the Ising model, as well as for the $q = 0$ case. The recent very precise calculation of the critical percolation probability p_c by Ziff and Suding [23] implies that neither conjecture is correct at $q = 1$, which is consistent with our observation at $q = 3$. The various estimates of w_c from numerical work and the conjectures by Wu and

Table 4. Numerical estimates for the critical point w_c of the Kagomé lattice Potts model, from this ($q = 3$ and 4) and other work ($q = 1$) [23] and exact results ($q = 2$) [24]. The lower bound w_{2b} is from King and Wu [6], while the conjectures are from Wu [3] and Tsallis [22].

q	w_c	w_{2b}	Wu	Tsallis
1	1.102 629(2)	1.071 0999...	1.102 7386...	1.093 6799...
2	$\sqrt{3+2\sqrt{3}}-1$	1.484 0238...	$\sqrt{3+2\sqrt{3}}-1$	$\sqrt{3+2\sqrt{3}}-1$
3	1.876 456(40)	1.793 1546...	1.876 2692...	1.889 5735...
4	2.156 1(5)	2.049 4407...	2.155 8422...	2.184 3871...

Tsallis are listed in table 4 together with recent exact lower bounds by King and Wu [6].

We have attempted to find an alternative conjecture within the framework of known results for other lattices, but without success. However, as our work excludes a large class of natural conjectures, it is worth reporting. It is also worth mentioning that the critical percolation probability p_c is known for site percolation on the Kagomé lattice, being equal to the corresponding result for bond percolation on the honeycomb lattice, $1-2\sin(\pi/18)$, which is in turn related to the critical percolation probability $2\sin(\pi/18)$ of bond percolation on the triangular lattice p_c. Indeed Tsallis uses this connection, and conjectures that p_c is given by

$$p^3 - p^2 - p + 1 - 2\sin(\pi/18) = 0 \tag{17}$$

which gives $p_c = 0.522\,37\ldots$. This disagrees with the recent numerical estimate of Ziff and Suding [23] by about 0.4%.

For the square, triangular and honeycomb lattices, the q-state Potts model critical point is given by the roots of a low-degree polynomial with (small) integer coefficients. These polynomials are:

$$y^2 - 2y - (q-1) = 0 \qquad \text{(square)} \tag{18}$$

$$y^3 - 3y + (2-q) = 0 \qquad \text{(triangular)} \tag{19}$$

$$y^3 - 3y^2 - 3(q-1)y - (q^2 - 3q + 1) = 0 \qquad \text{(honeycomb).} \tag{20}$$

In this form, $y = 1 + w$, and the root corresponding to $q = 0$ is $y = 1$ for all three lattices. For $q = 1$ (bond percolation) the root is $1/(1-p_c)$, for $q = 2$ it is $\exp(2J/kT_c)$, and for $q > 2$ it is $\exp(J/kT_c)$. If the co-ordination number of the lattice is z, then as q gets large, y behaves as $q^{2/z}$ for the three lattices.

In this form, the Wu conjecture can be written as

$$y^6 - 6y^4 + 2(2-q)y^3 + 3(3-2q)y^2 - 6(q-1)(q-2)y - (q-2)(q^2-4q+2) = 0. \tag{21}$$

For $q = 0$, this gives (correctly) $y = 1$. For $q = 2$ it simplifies to $y^6 - 6y^4 - 3y^2 = 0$, which gives the correct critical point for the Ising model, and as q gets large, y behaves, as expected, as $q^{1/2}$. However, the zero corresponding to $q = 1$ gives $p_c = 0.524\,4297\ldots$, which may be compared with the best numerical estimate $p_c = 0.524\,4053$, with uncertainty in the last quoted digit—that is to say, it is wrong, but by less than 0.005%. For $q = 3$ the relevant zero is $y = 2.876\,2692\ldots$, which may be compared with our best estimate of 2.876 46, with an error of no more than four in the last quoted digit. Again the conjecture is found to be wrong, but by a tiny amount, notably 0.007%. For $q = 4$ the appropriate zero is $3.155\,842\ldots$, while our estimate is 3.1561 ± 0.0005, which is indistinguishable from the conjectured zero. Thus the Wu conjecture is wrong, but is extraordinarily close

to the correct answers for all known values of q. The Tsallis conjecture for $q = 3$ is $y = 2.8895\ldots$, which is wrong by about 0.4%, as for $q = 1$.

We have attempted to find either a fourth-degree or a sixth-degree polynomial with q-dependent coefficients that reproduce all known results. In analogy with the results on other lattices, we required that the coefficient of the highest power of y be one, and that the coefficients be small integers (no more than $\pm$ 20). The coefficients are to be low-order polynomials in q. The large q behaviour noted above essentially restricts the degrees of these polynomials to quite low values. For any given value of q a large number of polynomials can be found, but the requirement that the coefficients be low-order polynomials in q has the consequence that we were unable to find any polynomial that met our requirements.

From this we conclude that no such polynomial exists (or that our search was not clever enough). This may even mean that the general result is not algebraic—though it clearly is for $q = 0$ and 2. This result is reminiscent of the absence of a believable conjecture for the site percolation threshold for the square and honeycomb lattices.

5. Summary and discussion

We have provided a radical extension of the low-temperature series for the q-state Potts model on the honeycomb ($q = 3$) and Kagomé ($q = 3$ and 4) lattices. An efficient implementation of the finite-lattice method, coupled with the prediction of additional terms has given rise to very long series. Our calculations were carried out on a single processor of a DEC ALPHA-SERVER 8400 with 1 Gb of memory per processor. Typical runs for the maximal width took 30 h per prime for $q = 3$ and 16 h for $q = 4$.

Analysis of these new series allowed us to give an estimate of the honeycomb lattice critical point which is entirely consistent with the presumed exact value. For the Kagomé lattice our results are inconsistent with any published conjectures, and our attempts to provide a more believable conjecture have been unsuccessful. We find no evidence for an algebraic critical point.

The pattern of dependence of estimates of u_c versus the known exponent for the honeycomb lattice, as shown in figure 5, is qualitatively similar to that found for the 3-state Kagomé lattice, and shown in figure 3. That is to say, the correct exponent underestimates u_c for the magnetization and susceptibility and overestimates u_c for the partition function and specific heat. Assuming this holds for the Kagomé lattice, it is gratifying to find that a consistent estimate of u_c emerges, notably $u_c = 0.347\,650(5)$, which we take as our final estimate.

Our extended series are likely to be of value in any further work on these problems. In particular, Maillard [20] has carried out an extensive investigation of the properties of the magnetization of the honeycomb lattice 3-state Potts model, and the results presented here should allow that work to be extended. We have also estimated the non-physical singularities, the properties of which are so informative, as shown recently by Matveev and Shrock [14].

Acknowledgments

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