

Low-temperature expansions for Potts models

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On simple-cubic lattices, we compute low-temperature series expansions for the energy, magnetization, and susceptibility of the three-state Potts model in $D=2$ and $D=3$ to 45 and 39 excited bonds, respectively, and the eight-state Potts model in $D=2$ to 25 excited bonds. We use a recursive procedure that enumerates states explicitly. We analyze the series with Dlog Padé analysis and inhomogeneous differential approximants.

Some of the present authors recently described a method^{1,2} similar to the finite-lattice method³ for generating low-temperature series for discrete models. This method is based on a recursive computer enumeration of configurations and has resulted in series expansions for the $D=3$ Ising model that extend available series by several terms.²⁻⁴

In this paper, we present results from a similar analysis for the low-temperature expansions of Potts models in two and three dimensions on a simple-cubic lattice. We will not describe the method used in much detail. It has already been outlined in Ref. 2 and will be described in detail in a separate paper.

The energy for the q -state Potts model is defined to be

$$E = \sum_{ij} (1 - \delta_{\sigma_i, \sigma_j}), \quad (1)$$

where σ_i is a site-defined field that takes q possible values. The sum is taken over all nearest-neighbor pairs of spins, with δ being the Kronecker symbol.

The partition function is the sum of the Boltzmann weights over all configurations,

$$Z = \sum_{\sigma} e^{-\beta E}. \quad (2)$$

Sorting configurations by energy, we rewrite this as a sum over E . Defining $P(E)$ to be the number of states with a given energy E , we have

$$Z = \sum_{E=0}^{dN} P(E) u^E, \quad (3)$$

where d is the number of dimensions, N is the number of sites, and $u = e^{-\beta}$.

We compute the coefficients $P(E)$ exactly on small systems by recursively assembling the system one site at a time. The method enables us to build up a lattice with arbitrary length in one direction. Intermediate stages require an explicit enumeration of exposed slices transverse to this direction. This effectively reduces the computational complexity to that of a system of one less dimension.

The starting point is a list of all states and corresponding energies for a single transverse layer of the lattice. In $D=2$ the transverse layer is a line of spins; in $D=3$ it is a plane of spins. All the spins outside this transverse layer are frozen to the same value; that is, the boundary conditions in the longitudinal direction are cold. Spins are then sequentially freed to build up the lattice in the longitudinal direction. We store the number of states with a

given energy E and the exposed top layer in an array $p_0(E, I)$, where the integer I is an index which specifies the exact configuration of the exposed transverse layer using bit coding. When a new spin is added, we obtain the new counts $p'_0(E, I)$ as a sum over the old counts, i.e.,

$$p'_0(E, I) = \sum_{I'} p_0[E - \Delta(I, I'), I'] . \quad (4)$$

Here I' can differ from I only in the bits representing the newly covered spins, and $\Delta(I, I')$ is the change in energy due to any newly changed bonds. For the present analysis we add the spins one at a time. Thus, the sum in the above equation is only over q terms, representing the q possible values of the newly covered spin. After the lattice is grown, a sum over the top layers gives the resulting $P(E) = \sum_I p_0(E, I)$. We always continue this recursion sufficiently to avoid finite-size errors in the longitudinal direction.

As the temperature goes to zero, so does the variable u . Thus, what we have in Eq. (3) is the low-temperature expansion for Z . From it we compute the series for the average energy, $\langle E \rangle = [u(\partial/\partial u)] \log(Z)$. Subtracting this expectation value before adding the last spin from its value after adding the last spin, we obtain the average energy per new site. This also eliminates the effect of the fixed end boundaries. Writing

$$(E/N) = \sum_j e_j u^j , \quad (5)$$

the low-temperature expansion amounts to listing the coefficients e_j .

The recursive technique can be extended to enable calculation of quantities such as the magnetization and susceptibility. We define a magnetization in the Potts model by

$$\langle M \rangle = \sum_i \langle \delta_{\sigma_i, 0} \rangle = N \sum_j m_j u^j , \quad (6)$$

assigning to each unexcited spin the value 1, and to each excited spin the value zero. The calculation of susceptibility is carried out using the fluctuation-dissipation theorem and we define the low-temperature series coefficients χ_j as follows:

$$N_\chi = \langle M^2 \rangle - \langle M \rangle^2 = N \sum_j \chi_j u^j . \quad (7)$$

Let $p(E, M, I)$ be the number of states with given energy, magnetization, and exposed top layer I . To compute any moment of the magnetization, it would be sufficient to compute $p(E, M, I)$. However, one can avoid computing this memory expensive quantity. Let us demonstrate this for the case of the magnetization.

First, note that $p_0(E, I) = \sum_M p(E, M, I)$ is the count we had before. To compute the magnetization, we need one more count: $p_1(E, I) = \sum_M M p(E, M, I)$. This is because the expectation value of magnetization can be written as

$$\langle M \rangle = \frac{\sum_E P_1(E) u^E}{Z} , \quad (8)$$

with $P_1(E) = \sum_I p_1(E, I)$ and $Z = \sum_{E, I} p_0(E, I) u^E$. The counting scheme for $p_1(E, I)$ is easy to derive. In analogy with Eq. (4) one can write

$$\begin{aligned} p'_1(E, I) &= \sum_M M p'(E, M, I) = \sum_{M, I'} M p(E - \Delta_e, M - \Delta_m, I') \\ &= \sum_{M, I'} (M - \Delta_m + \Delta_m) p(E - \Delta_e, M - \Delta_m, I') \\ &= \sum_{I'} [p_1(E - \Delta_e, I') + \Delta_m p_0(E - \Delta_e, I')] . \end{aligned} \quad (9)$$

Here $\Delta_e \equiv \Delta_e(I, I')$ and $\Delta_m \equiv \Delta_m(I, I')$ denote the change in energy and magnetization when adding the new spin. Thus, computation of the magnetization series requires just the introduction of one additional count (which only doubles the memory requirement) and we can calculate the magnetization series to essentially the same order as the energy series.

For the susceptibility series, we need to compute $\langle M^2 \rangle$. This requires a count $p_2(E, I) = \sum_M M^2 p(E, M, I)$. It is easy to see that p_2 obeys the recursion relation

$$\begin{aligned} p'_2(E, I) &= \sum_{I'} [p_2(E - \Delta_e, I') + 2\Delta_m p_1(E - \Delta_e, I') \\ &\quad + \Delta_m^2 p_0(E - \Delta_e, I')] . \end{aligned} \quad (10)$$

As discussed in Ref. 2, we work on generalized helical lattices and label our lattice points by their ordinal number on a helix. In three dimensions, the nearest neighbors on the lattice in the x , y , and z directions are separated by h_x , h_y , and h_z steps along the helix, respectively. We assume that the h 's are ordered so that $h_x < h_y < h_z$. Then, our numerical method requires us to keep track of, at most, q^{h_z} states and so we try to make h_z as small as possible. Let n be the effective lattice size, defined as the length of the shortest closed path on the helical lattice. For a given set of h values, if we compute the set of nonzero vectors $S = \{n_x, n_y, n_z; n_x h_x + n_y h_y + n_z h_z = 0\}$ then $n = \min S(|n_x| + |n_y| + |n_z|)$. The series expansion will be correct up to the order $u^{(4n-1)}$. Higher orders are corrupted by contributions from graphs that wrap around the lattice. However, as described in Ref. 2, we can combine results from different helical lattices to cancel these finite-size effects to some order in the series. In two dimensions, there is not enough complexity for this cancellation mechanism to work. Instead, one observes that keeping h_y spins in the top layer, the optimal choice of the lattice is $h_x = h_y - 1$. This gives the series correct to order $4h_y - 3$.

Our series are listed in Tables I–III. The series for $D=2$ and $D=3$ Potts models were computed on a CM-200/CM-2 connection machine using CM-FORTRAN and c* programs. The $D=2$, eight-states model series were computed on a CRAY-2 using a C code and checked on a CM-2 using CM-FORTRAN code. To obtain 3D series up to 39 excited bonds, we used lattices of effective size up to ten. This required the top layer to have at most 15 spins. In Table IV we show the lattices and combination factors used.

Note that our definition of M in Eq. (6) is such that in the completely disordered state it has the value N/q .

The proper order parameter for Potts models is the so-called reduced magnetization M_R which is related to M by the formula $M_R = (qM - N)/(q - 1)$. The reduced magnetization takes the values N and 0 in the completely ordered and disordered states, respectively. The results we give below from our analysis of series are for the reduced magnetization and the corresponding susceptibility.

In addition to the usual Dlog Padé (DIP) method,^{5,6} we will use the method of inhomogeneous differential ap-

proximants (IDA) introduced by Fisher and Au-Yang⁷ (see also Ref. 8). These are useful in handling singularities of the form

$$F(u) = A(u)(1 - u/u_c)^{\zeta} + B(u), \quad (11)$$

where A and B are analytic in u .

Given a series expansion for $F(u)$ to N th order, $F_N(u) = 1 + \sum_{i=1}^N f_i u^i$, (we will use the simplification that one can always normalize the series so that the constant

TABLE I. The low-temperature expansion coefficients e_i , m_i , and χ_i for the energy, magnetization, and susceptibility series for the $q=3$ Potts model in $D=2$ on a simple-cubic lattice.

i	e_i	m_i	c_i
0	0	1	0
1	0	0	0
2	0	0	0
3	0	0	0
4	8	-2	2
5	0	0	0
6	24	-8	16
7	28	-8	16
8	32	-24	100
9	216	-72	216
10	160	-140	844
11	660	-320	1552
12	2072	-1164	7844
13	1664	-1560	12112
14	11760	-7044	60268
15	17700	-13000	118944
16	41088	-35984	424072
17	156468	-101736	1081382
18	207240	-219616	3201728
19	849300	-647536	8670688
20	1817048	-1602194	25713154
21	4021780	-3970384	67206560
22	13178624	-11239056	203077760
23	25754296	-26891584	532881432
24	75653408	-73534214	1558159918
25	193458400	-191374464	4250639632
26	440725376	-486815472	11956293152
27	1296485460	-1323802480	33296697848
28	3009317200	-3380001144	92820406096
29	7977739920	-8964296480	257249275776
30	21217637824	-23766809488	721023458656
31	51359965976	-61628612552	1986080278600
32	140885970816	-165028619666	5561045323298
33	354038121756	-432231505864	15359165767512
34	916153258448	-1142608252368	42717426328784
35	2439917838708	-3039729276192	118457421095792
36	6161990034800	-7994207679356	328170466563836
37	16397314674708	-21295402476752	909829346983664
38	42540620667584	-56399959949412	2520622606225868
39	110314458936968	-149510058508096	6973368153491880
40	292427669006272	-398341255729746	19322697243220158
41	756553239055504	-1056154269407136	53409977638363032
42	1994873374110312	-2813530068950904	
43	5238354130103568	-7489714245193504	
44	13686401970717088	-19928407714223232	
45	36195015152016276	-53175417534052136	

term is unity), one computes coefficients for polynomials $Q_L(u) = \sum_{i=0}^L q_i u^i$, $R_M(u) = 1 + \sum_{i=1}^M r_i u^i$, and $S_J(u) = \sum_{i=0}^J s_i u^i$, which satisfy

$$F_N Q_L + S_J = F'_N R_M \quad (12)$$

to order N , with $L + M + J = N - 2$. Note that for $S_J = 0$, one obtains the usual Dlog Padé ratio from Q_L/R_M . It is easy to see that potential critical points u_c are the zeros of R_M and for each of these, the exponent ξ is estimated as $\xi = -Q_L(u_c)/R'_M(u_c)$.

Consider first the $D=2$ Potts models. Here, we know from self-duality that the critical point is at $u_c = 1/(\sqrt{q} + 1)$. For $q \leq 4$ the transition is continuous and the critical exponents are known exactly (see Ref. 9 and references therein). Models with $q > 4$ undergo a first-order phase transition. Having results from both of the above categories available, our $D=2$ series offer themselves as a good testing ground for series analysis methods.

Given the low-temperature series, does one have enough information to determine the nature of the transition, assuming that the critical temperature is exactly known? In $D=2$, because of self-duality, this is easy if the series at hand has a sufficient number of terms. To illustrate this, we plot in Fig. 1(a) the energy as a function of u from the low-temperature series and its dual high-temperature series for $q=3$ and $q=8$. In Figs. 1(b) and 1(c) we plot the latent heat $L(n)$ derived using duality at the known critical point as a function of the number of

terms n in the series. The fits of L to a power law in $1/n$ [Figs. 1(b) and 1(c)] convincingly demonstrate that the $q=3$ model has a second-order transition while the $q=8$ model has a first-order transition with the latent heat equal to $\frac{1}{2}$ to 2 parts/ 10^3 .

In general however, self-duality is not available as a symmetry. In this case, one must rely on DIP and IDA analyses on the low-temperature series to determine the critical properties. Our arguments below are similar in spirit to the discussion presented by Enting and Guttmann.¹⁰

If the system undergoes a second-order phase transition, one expects, in general, that the order parameter M_R/N vanishes at the critical point, approaching it with infinite slope. Estimates of the critical temperature (poles) from DIP should then cluster well around the exact value and estimates of the critical exponent β (residues) should also be quite accurate. On the other hand, at a first-order transition, the magnetization is finite and nonzero and its slope can be either finite or infinite. In this case one would expect the approximants to continue the curve beyond the critical temperature along the so-called pseudospinodal line.¹¹ This line intersects the temperature axis at the point u_S with corresponding exponent β_S . Applying DIPs in this case should then result in a systematic overestimation of the critical temperature because it is u_S that the Padé is trying to fit.

In the case of a first-order transition with a divergent slope of the magnetization as the transition is approached, DIPs still tend to overestimate the transition

TABLE II. The low-temperature expansion coefficients e_i , m_i , and χ_i for the energy, magnetization, and susceptibility series for the $q=8$ Potts model is $D=2$ on a simple-cubic lattice.

i	e_i	m_i	c_i
0	0	1	0
1	0	0	0
2	0	0	0
3	0	0	0
4	28	-7	7
5	0	0	0
6	84	-28	56
7	588	-168	336
8	-588	91	0
9	4536	-1512	4536
10	11760	-4060	14504
11	-13860	0	15792
12	2050172	-68859	288169
13	144144	-84840	556752
14	271460	-256424	2062088
15	7553700	-2678760	15132264
16	-713692	-2049229	25582802
17	45219048	-21023016	165495792
18	232853880	-93466856	720185368
19	-14850780	-107162496	1588846728
20	2822644748	-1187630969	10588862669
21	6212314080	-3159741984	33856668720
22	8166041884	-7756117236	108773186200
23	131708763816	-56277329304	596266427232
24	167481870528	-118516443339	1709093729238
25	846878642400	-506752816584	7126592218032

TABLE III. The low-temperature expansion coefficients e_i , m_i , and χ_i , for the energy, magnetization, and susceptibility series for the $q=3$ Potts model in $D=3$ on a simple-cubic lattice.

i	e_i	m_i	χ_i
0	0	1	0
1	0	0	0
2	0	0	0
3	0	0	0
4	0	0	0
5	0	0	0
6	12	-2	2
7	0	0	0
8	0	0	0
9	0	0	0
10	60	-12	24
11	66	-12	24
12	-168	28	-56
13	0	0	0
14	420	-90	270
15	900	-180	540
16	-1728	318	-930
17	-2448	432	-1296
18	6708	-1320	4768
19	9462	-1992	7968
20	-14280	2760	-10560
21	-49686	9368	-36992
22	71940	-14460	64812
23	177192	-35280	163440
24	-194544	36680	-165464
25	-684300	134568	-659088
26	515892	-108516	600024
27	3087234	-609692	3278256
28	-1927296	370500	-1980408
29	-10943904	2153016	12285816
30	3863712	-792218	5005014
31	44383506	-8867580	55200864
32	-4406976	935124	-6062712
33	-177069948	34889512	-227203096
34	-1133220	63834	1954650
35	652560090	-130265472	914339736
36	199263288	-39322372	
37	-2553456210	507892056	
38	-1235636652	239776590	
39	9742992324	-1940344524	

TABLE IV. The lattice parameters and combination factors that give the series accurate to 39 excited bonds in $D=3$.

h_x	h_y	h_z	Coefficient
9	14	15	2
11	12	15	-1
9	11	15	-2
10	13	14	1
11	12	14	5
9	11	14	-1
7	12	13	1
10	11	13	-3
8	10	13	1
5	11	12	3
7	10	12	-5

point because the finite value of the magnetization is not modeled in the DIPs (more detailed reasons can be found in Ref. 12). However, for this case, the IDAs should treat the situation better because they can account for a finite $\langle M/N \rangle$ at the critical point. Thus, comparing the results of the two types of approximants, one might be able to determine the order of the transition.

Applying DIPs to the 45-term magnetization series of the three-state model in $D=2$ leads to a slight systematic underestimation of the critical point. Taking into account seven most central approximants we obtained $u_c = 0.36595 \pm 0.00003$, which is to be compared with the exact value $u_c = 0.36602 \dots$. The error here corresponds to the scattering of values from the different DIPs. In the light of the above discussion, this suggests that the

transition is continuous. We estimate the critical exponent $\beta=0.1084\pm 0.0002$ by evaluating it at the known critical point for this model. The error bar is meaningless, of course, as it comes only from the error on the extrapolation and ignores the systematic effects of the finiteness of the series. The value obtained is about 2.5% below the exact result $\beta=\frac{1}{9}$.

In the eight-state model in $D=2$, on the other hand, DIPs show a critical point at $u_c=0.2628\pm 0.0003$, which is substantially beyond the true value $u_c=0.2612\dots$. This suggests a first-order phase transition. In Fig. 2 we plot u_c vs β for small values of J . The points for different J lie fairly well on a line with an obvious tendency to

overestimate the critical point. This again establishes the first-order nature of the transition. The corresponding pseudoexponent estimated from DIPs has the value $\beta_S=0.059\pm 0.005$.

Similar ideas can be applied to the energy and specific-heat series. At a first-order phase transition there is a finite latent heat but the energy curve can have either finite or infinite slope (specific heat) as that point is approached. DIP analysis of the $q=3$ specific-heat series in $D=2$ shows a slight overestimate of the critical point, namely $u_c=0.36626\pm 0.00001$. IDAs, on the other hand, lead to a small underestimate (see Fig. 3) giving an overall consistency with the second-order phase transi-

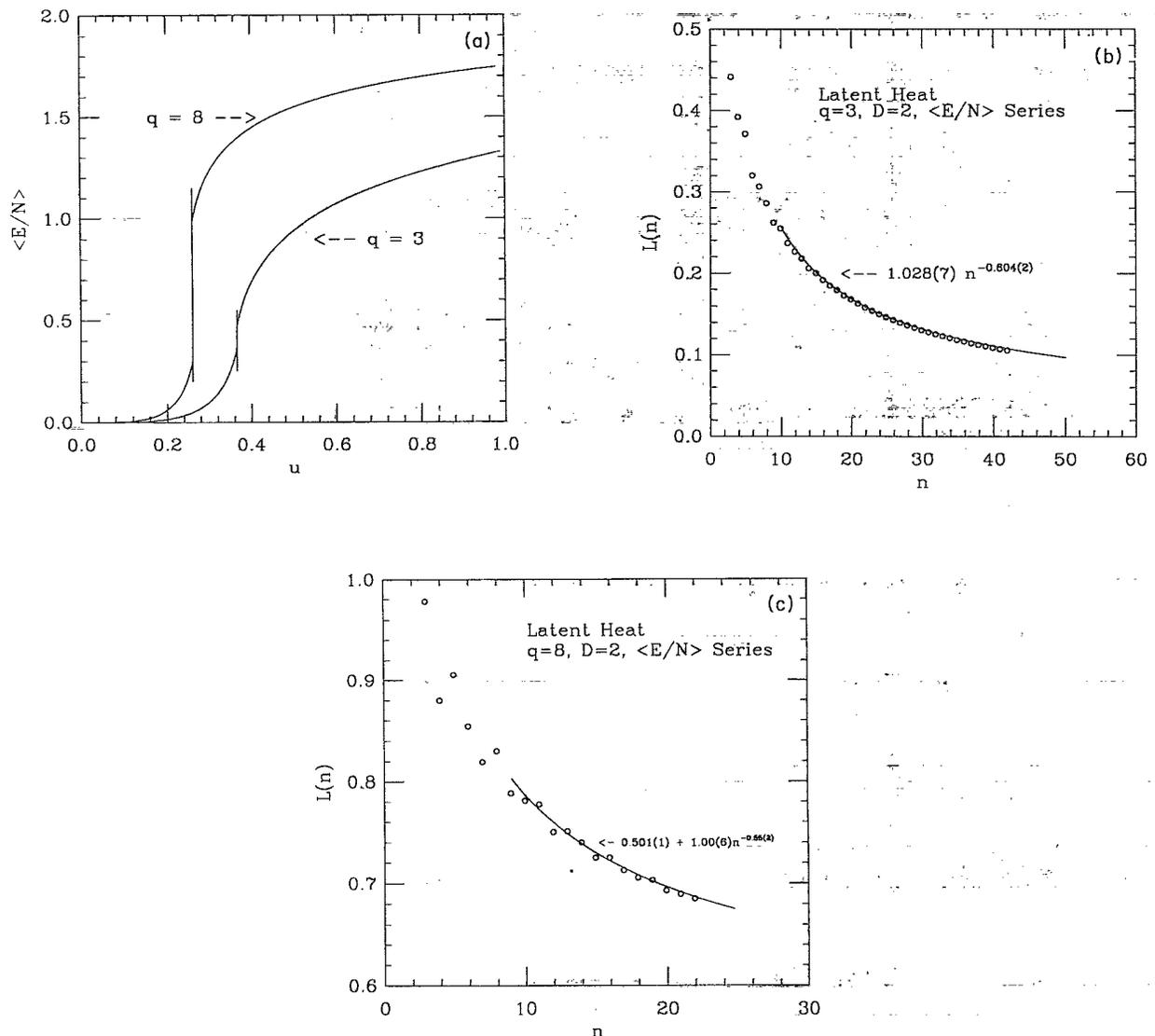


FIG. 1. (a) The average energy from the series expansions in $D=2$ for $q=3$ and $q=8$. Duality was used to get the series in the high-temperature phase from the series in the low-temperature phase. The exactly known transition points are shown as vertical lines. (b) The latent heat $L(n)$ as a function of n for $q=3$ in $D=2$. The solid line is a fit to a power law and demonstrates that for $n = \infty$, the latent heat vanishes. (c) The latent heat $L(n)$ as a function of n for $q=8$ in $D=2$. The solid line is a fit to a power law plus a constant and demonstrates that for $n = \infty$, the latent heat is about $1/2$.

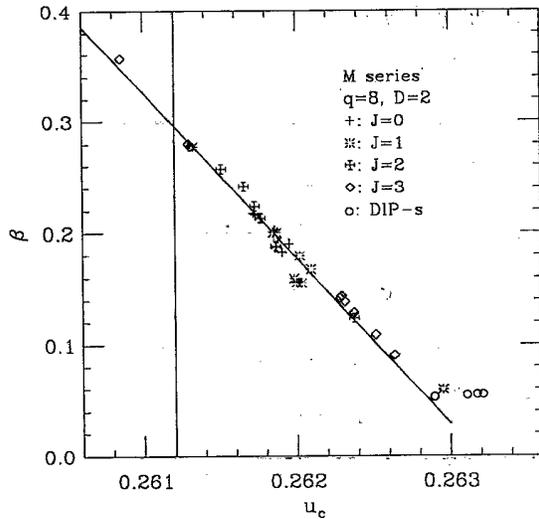


FIG. 2. u_c vs the exponent β from the magnetization series for the $q=8$ model in $D=2$. The exact value of u_c is the vertical line.

tion present. DIPs average for critical exponent $\alpha=0.412\pm 0.001$ is rather poor when compared to the exact value $\alpha=1/3$. This is probably due to the strong confluent singularity present in this case.¹³ The results of the IDA analysis is shown in Fig. 3 where we plot u_c vs α for various J comes from 0–20 with L and M chosen to be equal or differing by, at most, 1 [see Eq. (12)]. Notice that if we fit the data to a straight line and compute the value of α at the exactly known critical point (vertical line in Fig. 3), we obtain a result which differs from the exact value by about 1%.

In the $q=8$ model, the results from the specific-heat series and magnetization series are very consistent with each other. There is an overestimate of the critical point by DIPs ($u_S=0.2620\pm 0.0001$) as well as by IDAs. The

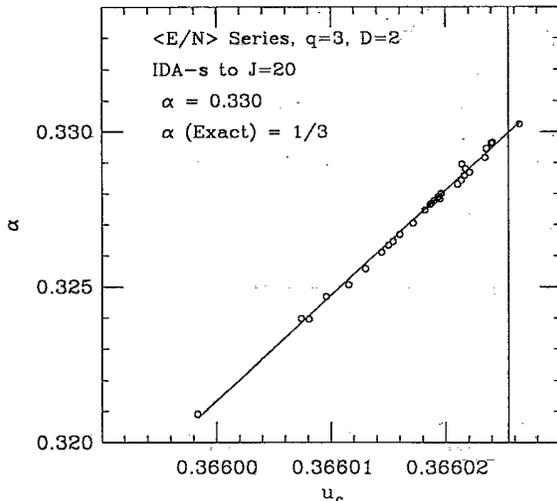


FIG. 3. u_c vs the exponent α from the series for the specific heat for $q=3$ in $D=2$ from IDA analysis. The vertical line is the exact value of u_c .

averaged pseudoexponent from DIPs is $\alpha_S=0.592\pm 0.004$.

Finally, an analysis of the susceptibility series for the $q=3$ model using the Dlog Padé and IDA analyses gave $\gamma=1.47\pm 0.02$ by extrapolating to the known critical point, as was done above for α and β . This is to be compared with the exact result $\gamma=13/9=1.444\dots$. For the $q=8$ model, we estimate $u_S=0.2629\pm 0.0009$, $\gamma_S=1.16\pm 0.07$.

Let us now turn to the series for the $q=3$ Potts model in $D=3$, given in Table III. Theoretically, this is the most interesting case of these considered in this paper, because of its connection to the SU(3) lattice gauge theory in $D=4$ (Ref. 14) and because of the lack of any exact results. There was a good deal of confusion about the nature of the transition in the past but by now the first-order nature of this transition seems to be well established.¹⁵ Although the transition temperature is not known exactly, there are very accurate Monte Carlo estimates for it. For the purpose of our analysis we will assume that the value $u_c=0.57659(1)$ estimated in Ref. 15 is the exact result. We will do so because we found that neither the DIP nor the IDA analyses can yield a more accurate value.

Consider first the magnetization series. In Fig. 4 we show the results from central Dlog Padés. The data cluster well around the value $u_c=0.5785\pm 0.0003$, quite far from 0.57659. IDAs show the same tendency as can be seen in Fig. 5. Here, the results from small J fall very nicely on a straight line beyond the critical point which is marked by a cross. These results support the conclusion that this model has a first-order phase transition in agreement with Ref. 10 and Monte Carlo data.¹⁵ The critical pseudoexponent from DIPs has the value $\beta_S=0.204\pm 0.002$, which agrees very accurately with results of Miyashita, Betts, and Elliot¹⁶ who analyzed a shorter series, and also with numerical simulations.¹⁷

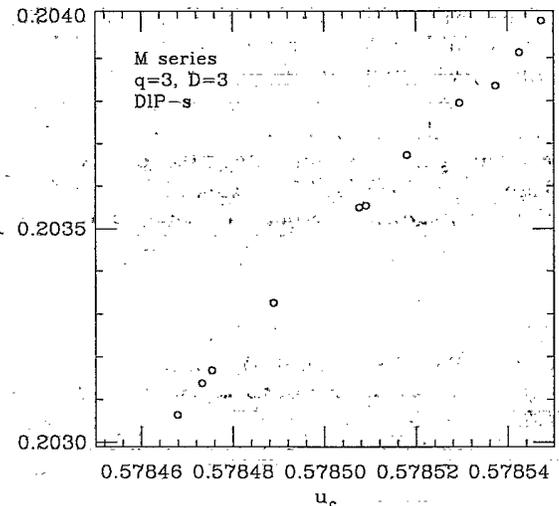


FIG. 4. u_c vs the exponent β from the magnetization series for the $q=3$ model in $D=3$ using DIPs.

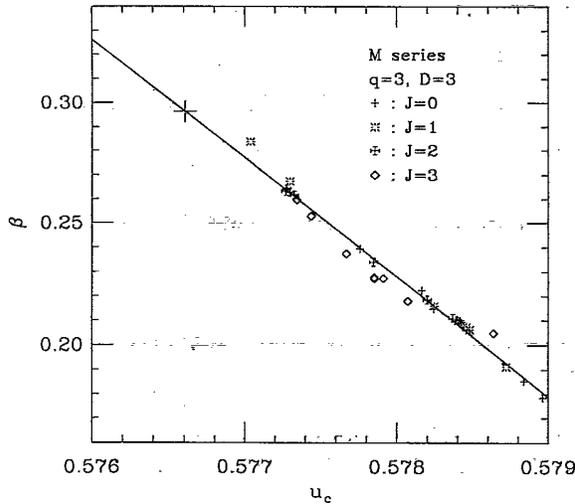


FIG. 5. u_c vs the exponent β from the magnetization series for the $q=3$ model in $D=3$ using IDAs with small J values. The exact value of u_c is marked with a plus and is a Monte Carlo result from Ref. 15.

Next consider the specific-heat series. Here one obtains stable results from many central Dlog Padés. Also, the IDAs are quite stable for small J . Figure 6 shows the results of these analyses. The circles correspond to the DIPs and the other symbols are the results from the IDAs for $J \leq 4$. There is no clear evidence for systematic overestimation of the critical point by either DIPs or IDAs, suggesting that the transition is weakly first order in this variable. The straight lines in Fig. 6 are least-square fits to IDAs and DIPs. Since the latent heat is small, one would expect that these should intersect at the critical point where they are both dominated by the singularity. Away from the critical point, the Dlog Padé and the IDAs treat the nonleading corrections differently and so the results from them could be different. Indeed, the lines in Fig. 6 intersect at $u_c = 0.5766(2)$, $\alpha = 0.421(2)$. We have estimated the error on these parameters from the errors in the fitted parameters for the straight lines.

Finally, we analyzed the $q=3$ susceptibility series in three dimensions. Here the combined data for DIP and IDA fall nicely on a line. We estimate $\gamma = 1.085 \pm 0.005$ by evaluating the fitted line at $u_c = 0.57659$.

Recently, Vohwinkel¹⁸ has extended the shadow lattice method and shown how one can obtain extremely high-

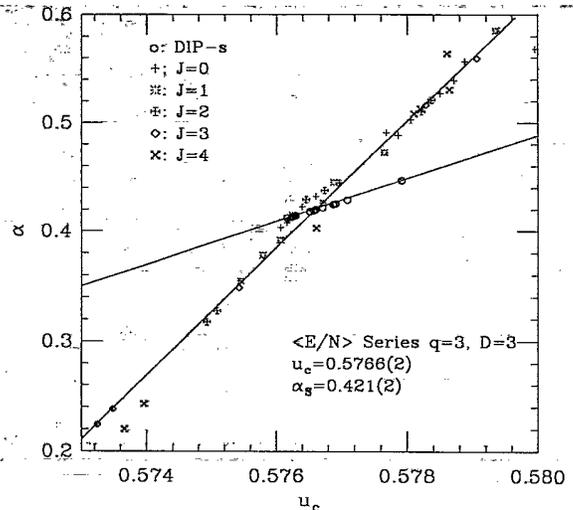


FIG. 6. u_c vs the exponent α from the series for the specific heat for $q=3$ in $D=3$ from DIP and IDA analysis. The transition point is accurately determined by the crossing of the lines for DIPs and IDAs.

order low-temperature expansions. His series for the magnetization has several more terms than ours and although he does not generate series for the other quantities we measure in the present paper, we presume he can do so. A challenge now is to see if the ideas of Ref. 18 can be incorporated into our method.

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