High-temperature series expansions for the q-state Potts model on a hypercubic lattice and critical properties of percolation

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We present results for the high-temperature series expansions of the susceptibility and free energy of the q-state Potts model on a D-dimensional hypercubic lattice $\mathbb{Z}^D$ for arbitrary values of q. The series are up to order 20 for dimension $D \leq 3$, order 19 for $D \leq 5$, and up to order 17 for arbitrary D. Using the $q \to 1$ limit of these series, we estimate the percolation threshold p_c and critical exponent γ for bond percolation in different dimensions. We also extend the $1/D$ expansion of the critical coupling for arbitrary values of q up to order D^{-9}.

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I. INTRODUCTION

Since many years the q-state Potts model [1] has served as paradigmatic system for the study of phase transitions and critical phenomena. Fortuin and Kasteleyn reformulated it as a random cluster model in which q appears as a general parameter no longer restricted to $q=2,3,\ldots$ and where bond percolation appears as the special case $q=1$.

Systematic series expansions have a long history [2] as a method to analyze lattice models of phase transitions. In the case of Potts models, high-temperature series for the susceptibility and free energy with q as a free parameter have been obtained for D-dimensional hypercubic lattices in Ref. [3] (free energy only) and Ref. [4]. We extend these series considerably and use them for a scan of the phase diagram in (q,D) space. A detailed analysis is presented for the case of bond percolation $(q=1)$ on higher-dimensional hypercubic lattices, extending the analysis of 15th order percolation series in arbitrary dimensions of Ref. [5].

We shortly review the model and its cluster formulation in Sec. II and the star-graph expansion technique in Sec. III. In the following sections we present results for general parameter q in two (Sec. IV) and higher (Sec. V) dimensions. Section VI treats the large-dimensionality expansion of the critical coupling, and in Sec. VII the case of bond percolation, i.e., the limit $q=1$, is analyzed. We end with a short summary in Sec. VIII.

II. THE q-STATE POTTS MODEL

Let $G=(V,E)$ be an undirected graph, that is a set V of vertices together with a set E of edges defining which pairs of vertices are considered "nearest neighbors." Put a spin s_i on each vertex $i \in V$ which can take q different values. The q-state Potts model (see, e.g., Ref. [1] for a review) on this graph is then defined by the Hamiltonian

$$H = -J \sum_{(ij)\in E} \delta(s_i,s_j), \tag{1}$$

where $\delta(\cdots)$ is the Kronecker δ symbol. The Fortuin-Kasteleyn representation shows that the partition function $Z_G=\Sigma_{\{s_i\}} e^{-\beta H}$ for a finite graph G is actually a polynomial in q and $w=e^{\beta J}-1$:

$$Z_G(q,w) = \sum_{C\subseteq E} q^{N_c(C)} w^{|C|}. \tag{2}$$

Here the sum is over all $2^{|E|}$ clusters, i.e., subsets C of the set E of edges; $N_c(C)$ is the number of connected components, where each isolated vertex is counted as one component, and $|C|$ is the number of edges of C. This allows one to study the model for arbitrary values of $q \notin \{2,3,\ldots\}$ which can no longer be represented by a local interaction of spin degrees of freedom of the original Hamiltonian (1). Of special interest in statistical physics are the limits $q \to 1$ and $q \to 0$ which can be shown to be related to percolation and tree percolation on the graph G, respectively.

A two-point correlation function can be defined in the cluster representation simply by

$$D(i,j) = \frac{1}{Z_G} \sum_{C_{ij}\subseteq E} q^{N_c(C)} w^{|C|}, \tag{3}$$

where the cluster sum is restricted to those clusters C_{ij} in which the vertices i and j belong to the same connected component. The susceptibility related to this correlator,

$$\chi_G(q,w) = \frac{1}{|V|} \sum_{i,j\in V} D(i,j), \tag{4}$$

equals for $q=2,3,\ldots$ the usual magnetic susceptibility of the q-state Potts model in the high-temperature phase (i.e., as long as $\langle s_i \rangle = 0$).

In the case $q=1$ the weight of a cluster in the partition sum depends only on its number of edges. This case therefore describes bond percolation where the local bond

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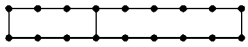
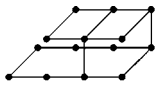


$$7620\binom{D}{2} + 76851600\binom{D}{3} + 14650620864\binom{D}{4} + 404500471680\binom{D}{5} + 3355519311360\binom{D}{6}$$



$$12048\binom{D}{3} + 396672\binom{D}{4} + 2127360\binom{D}{5} + 2488320\binom{D}{6}$$

FIG. 1. Two star graphs of order 19 (left) and 17 (right) and their weak embedding numbers. Due to its topology, the result is complete (valid for arbitrary dimension D) for the graph of order 17. For the graph of order 19 it is valid only up to $D=6$.

probability is given by $p=w/(w+1)$. It easily follows that here the susceptibility $\chi(q=1,w)$ measures the average size of the percolation cluster.

The Potts partition function $Z_G(q,w)$ is essentially equivalent to the Tutte or dichromatic polynomial of the graph G, see, e.g., Ref. [6] and references therein. It encodes a lot of combinatorical properties of the graph such as the number of spanning trees, the number of spanning forests, the number of possible acyclic orientations, or the number of vertex colorings with q different colors using different colors on neighboring vertices. The last mentioned number, for example, equals $\lim_{\beta J\to-\infty} Z_G(q,e^{\beta J}-1)=Z_G(q,-1)$, which is the number of ground states of the antiferromagnetic q-state Potts model on the graph G.

In statistical physics, on the other hand, the interest in these models is related to the existence of a phase transition between a disordered high-temperature (low-density in the case of percolation clusters) and an ordered low-temperature (large w) phase if we go to infinite graphs like the D-dimensional hypercubic lattice $G=\mathbb{Z}^D$. Depending on q and D, these transitions can be first or second order. Whereas in $D=2$ dimensions many exact results are available showing that the second-order nature changes to first-order for $q>4$, in $D=3$ and higher dimensions there is strong numerical evidence that the transition is of first order for all integer values $q>2$. In the case of a second-order phase transition at β_c, the behavior of the susceptibility (4) is characterized by the critical exponent γ: $\chi_G\sim|\beta-\beta_c|^{-\gamma}$.

III. HIGH-TEMPERATURE SERIES EXPANSIONS

Series expansions are an important tool for the extraction of information on statistical systems which is exact (up to the order of the expansion) in the thermodynamic limit. There exist different well-established methods [2] for the systematic generation of high-temperature series expansions, as for example the linked cluster and the star-graph method. The latter one received its name from the fact that only one-vertex-irreducible graphs contribute to the series. In an attempt to study systems with quenched disorder via series expansions [7–11] we used this method and developed a comprehensive software toolbox for generating and enumerating star graphs which is reused in this work.

The basic idea of the star-graph method is to assemble the value of some extensive thermodynamic quantity F on a large or even infinite graph from its values on subgraphs: Graphs constitute a partially ordered set under the "subgraph" relation. Therefore, for every function $F(G)$ defined on the set of graphs exists another function $W_F(G)$ such that for all graphs G,

$$F(G)=\sum_{g\subseteq G} W_F(g), \tag{5}$$

and this function can be calculated recursively via

$$W_F(G)=F(G)-\sum_{g\subset G} W_F(g). \tag{6}$$

This gives for an infinite, e.g., hypercubic, lattice

$$F(\mathbb{Z}^D)=\sum_G (G:\mathbb{Z}^D)\, W_F(G), \tag{7}$$

where $(G:\mathbb{Z}^D)$ denotes the weak embedding number of the graph G in the given lattice structure [12].

The following observation makes this a useful method: Let G be a graph with an articulation vertex where two star subgraphs $G_{1,2}$ are glued together. Then $W_F(G)$ vanishes if

$$F(G)=F(G_1)+F(G_2). \tag{8}$$

An observable F for which Eq. (8) is true on arbitrary graphs with articulation points allows a star-graph expansion. Then all nonstar graphs have zero weight W_F in the sum of Eq. (7). It is easy to see that the (properly normalized) free energy $\ln Z$ has this property and it can be shown that the inverse susceptibility $1/\chi$ has it, too.

The weak embedding numbers $(G:\mathbb{Z}^D)$ of a graph G into the hypercubic lattice are counted using a refined version of the backtracing algorithm by Martin [12], making use of a couple of simplifications for bipartite hypercubic lattices $\mathbb{Z}^D$. Figure 1 shows two typical results. A star graph of order n can use at most $\lfloor\frac{n}{2}\rfloor$ dimensions of the lattice and every embedding using m dimensions appears in $\mathbb{Z}^D$ with multiplicity $\binom{D}{m}$.

For the symbolic calculations of the partition sum and susceptibility on every star graph up to a given order (ca. 80 000 up to order 20) as polynomials in q and w, we developed a C++ template library using an expanded degree-sparse representation of polynomials and series in many variables. The open source "Multiple Precision Arithmetic Library (GMP)" is used for the arbitrary-precision arithmetics. Our series for the free energy $\ln Z$ and the susceptibility χ with q as a free parameter are up to order 20 for dimension $D\leq 3$, order 19 for $D\leq 5$, and up to order 17 for arbitrary D.

In order to check our algorithms we did a careful comparison with older published series data. Our series agree with the 10th order susceptibility and free energy series for arbitrary q and D of Ref. [4] (modulo some misprints in their expression for $\ln Z$) as well as with the 16th order $D=2$ free energy series of Ref. [3], but disagree in several places with the 11th order, arbitrary dimension free energy series in the last mentioned paper. For the special case of bond percolation $q=1$ they agree with the 15th order arbitrary-dimension series of Ref. [5]. In the special case of the three-dimensional Ising model ($q=2$, $D=3$) our 20th order series also conform with the 25th order series of Ref. [13] generated by linked-cluster expansion. They also agree with the 21st order

$q=3, D=3$ partition function series of Ref. [14] obtained by finite lattice methods. In two dimensions, much longer series exist for special models. Our 20th order susceptibility series agree with the $q=3$ and $4, D=2$ series of Ref. [15].

We close this section with some remarks about the analysis of the thus generated expansions. The estimate of critical parameters from a high-temperature series involves extrapolation from a finite number of exactly known coefficients to the asymptotic form of the function. Many such extrapolation techniques have been developed and tested for different series and are comprehensively reviewed in Ref. [16]. These extrapolation techniques are not rigorous. They make some assumptions about the expected form of the singularity at the critical temperature. Usually, error estimates rely on the scatter of the results of extrapolations with different parameters (like $[N/M]$ Padé approximants for different values of N and M). This may seriously underestimate systematic errors coming from wrong assumptions about the structure of the singularity.

In order to obtain a reliable picture, we will take into account several criteria, such as (a) convergence of the analysis, (b) scatter of different approximants, (c) number of defective approximants, and (d) agreement between different extrapolation methods.

The basic methods we use are Dlog-Padé approximation and inhomogeneous differential approximants (IDA) [16]. In order to analyze confluent nonanalytic and logarithmic corrections, these methods are applied to suitably transformed forms of the series. The parameters of these transformations are fine tuned according to the criteria listed above, a technique pioneered in Ref. [5].

IV. TEST: TWO DIMENSIONS

The Potts model in two dimensions is exhaustively reviewed in Ref. [17]. We repeat here the principal facts: Baxter has determined the exact free energy on $\mathbb{Z}^2$ along the two curves

$$w_F = \sqrt{q}, \tag{9}$$

$$w_A = -2 + \sqrt{4-q}, \tag{10}$$

in (q,w) parameter space. The curve (9) gives the locus of the ferromagnetic phase transition and is perfectly understood in terms of conformal field theory. Critical exponents are exactly known, e.g.,

$$\gamma = \frac{4+3k^2}{12k-6k^2}, \quad \text{where } \sqrt{q} = -2\cos(\pi/k). \tag{11}$$

The curve (10) is conjectured to be the locus of the antiferromagnetic transition which agrees with the known facts for $q=2,3,4$.

A thorough analysis of the susceptibility series of order 20 using Padé approximants to the logarithmic derivative of the susceptibility (Dlog-Padé approximants) is shown for the ferromagnetic case in Figs. 2 and 3 where around 15–25 different $[N/M]$ approximants are plotted for each value of q. The continuous lines present the exact results (9) and (11). We find a quite satisfactory agreement also for noninteger values of q, however, the scatter of different approximants and the number of defective approximants increases for smaller values of q. This may be related to the fact that the $q \to 0$ limit is a quite intricate multicritical point [17].

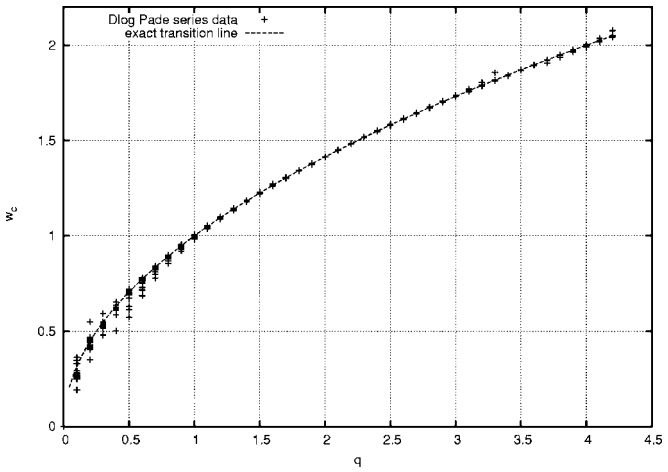


FIG. 2. Critical coupling w_c as function of q in two dimensions.

V. HIGHER DIMENSIONS: OVERVIEW

The explicit q and D dependence of our series allows us to obtain a fast overview over the phase structure in a large parameter range. Figures 4 and 5 show the results of a Dlog-Padé analysis of the susceptibility series for the critical coupling $v=(e^{\beta J}-1)/(e^{\beta J}-1+q)=w/(w+q)$ and exponent γ.

Several remarks are in order:

(i) At the upper critical dimension ($D=4$ for $q=2$, $D=6$ for $q=1$) the Dlog-Padé analysis finds a value $\gamma \approx 1.08$ slightly larger than 1. This effect is well known and due to the existence of logarithmic corrections.

(ii) For $D \geq 3, q \geq 3$ the phase transition is of first order and the correlation length remains finite. In analyzing high-temperature series by Padé approximants or similar techniques, the approximant will provide an analytic continuation beyond the first-order transition temperature T_0 into a metastable region on a pseudospinodal line with a singularity $T_c^* < T_0$ and effective exponents at T_c^*. Our v_c in this region is therefore an upper bound of the real transition point.

(iii) For $D=3$, the curve $\gamma(q)$ passes $\gamma=1$ at $q \approx 2.7$, marking the onset of a first-order transition. This is consistent with slightly smaller estimates in the literature coming from Monte Carlo computer simulations and field theoretic calculations (see Ref. [18] and references therein). It would be interesting to see if the crossover point can be understood as a kind of tricritical point in the (q,v) parameter space.

Since high-temperature series alone are not sufficient to analyze first-order transitions (and much longer series exist for the special case of the three-dimensional Ising model $q=2, D=3$), we concentrate our analysis in the second part of the paper on the $q=1$ case of bond percolation.

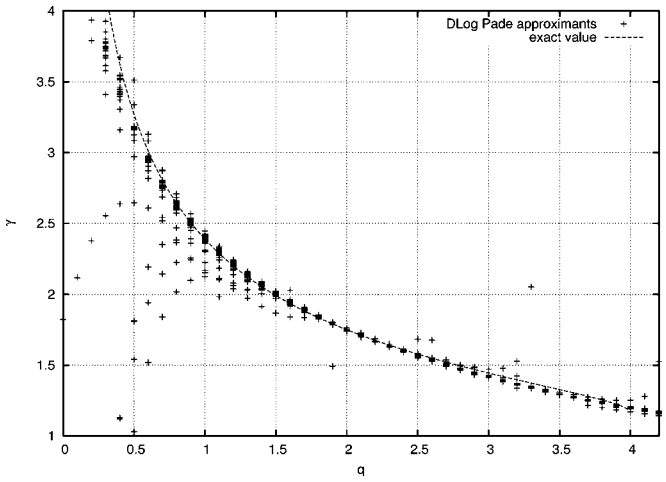


FIG. 3. Critical exponent γ as function of q in two dimensions.

VI. LARGE-DIMENSIONALITY EXPANSION

The dimension of the lattice enters the star-graph series expansion only through the embedding numbers [Eq. (7)] and we keep it as a free parameter in our series (see Fig. 1). This allows one [19] to extract a large-D expansion for the critical coupling from the susceptibility series by iteratively solving the critical point equation $1/\chi(D,v_c)=0$ in terms of v_c as series in $1/D$. This gives the large-D expansion of v_c up to order D^{-n} if χ is known as series in v up to order $2n$. For the $O(N)$ model the first terms of the $1/D$ expansion of the critical coupling for arbitrary N were obtained by Gerber and Fisher [20], who also demonstrated by solving the large N limit that this expansion is only asymptotic.

As far as we know, our analogous series for the q-state Potts model with arbitrary q is new. For the percolation ($q=1$) case the first five orders were calculated in Ref. [21]. We give the series for v_c in terms of the branching number σ which is one less than the coordination number of the lattice and therefore for the hypercubic lattice $\sigma=2D-1$,

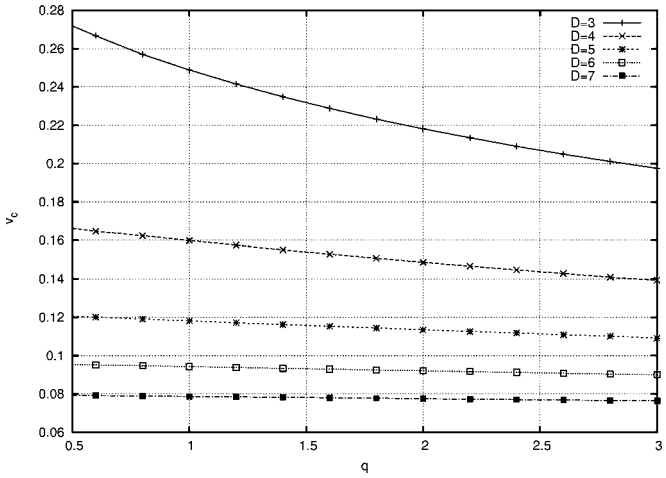


FIG. 4. Critical coupling v_c as function of q in different dimensions.

$$v_c(q,\sigma)=\frac{1}{\sigma}\Bigg[1+\frac{8-3q}{2\sigma^2}+\frac{3(8-3q)}{2\sigma^3}+\frac{3(68-31q+q^2)}{2\sigma^4}+\frac{8664-3798q-11q^2}{12\sigma^5}+\frac{78768-36714q+405q^2-50q^3}{12\sigma^6}+\frac{1476192-685680q-2760q^2-551q^3}{24\sigma^7}+\frac{7446864-3524352q-11204q^2-6588q^3-9q^4}{12\sigma^8}+\cdots\Bigg]. \tag{12}$$

By using σ as the expansion variable we see that the first correction to the Bethe lattice result $v_c=1/\sigma$ is absent for all values of q. Figure 6 shows plots of the critical coupling as obtained from Eq. (12) by simply summing up all terms. Since these expansions are asymptotic series, for relatively small D a more careful treatment with appropriately adapted maximal order would actually be necessary, as discussed below for the percolation case $q=1$. Of course, in the case of first-order phase transitions, the expansion (12) yields the pseudospinodal transition point in the metastable region.

VII. $q\to 1$: PERCOLATION

The $q\to 1$ limit of the Potts model describes bond percolation with local bond probability $p=w/(w+1)=v$. Standard scaling theory [22] describes the number of clusters of size s for large s near the percolation threshold p_c by

$$n(s,p)\sim s^{-\tau}f\left((p_c-p)s^{\sigma}\right), \tag{13}$$

introducing a scaling function f and the critical exponents τ and σ. The $q\to 1$ limit of the Potts model susceptibility describes the average cluster size and $\frac{\partial \ln Z}{\partial q}$ the number of clusters. Their respective critical exponents are related to the scaling law equation (13) by

$$\gamma=\frac{3-\tau}{\sigma}, \tag{14}$$

$$2-\alpha=\frac{\tau-1}{\sigma}. \tag{15}$$

A thorough analysis of percolation series in higher dimensions was done some years ago in Ref. [5]. Since we extended the series from 15 to 17 (for $D\geq 6$), 19 (for $D=4,5$), and 20 (in $D=3$) terms, a careful reanalysis seems to be in place (for extensive percolation series expansions in two dimensions, see Ref. [23] and, recently, Ref. [24]).

A. Up to the upper critical dimension

The divergence of the susceptibility (mean finite cluster size) is expected to be of the form

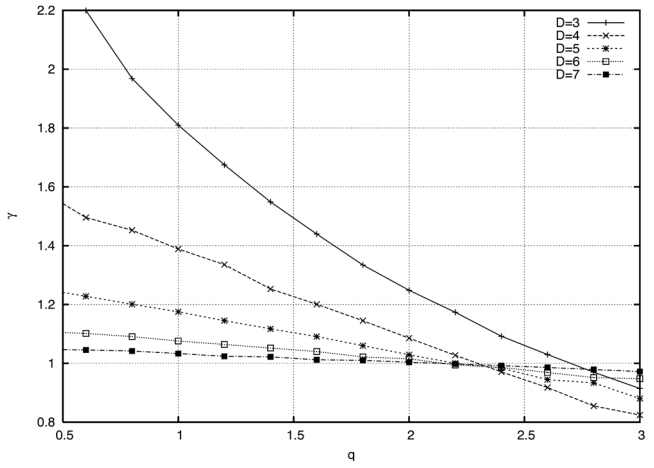


FIG. 5. (Color online) Critical exponent γ as function of q in different dimensions.

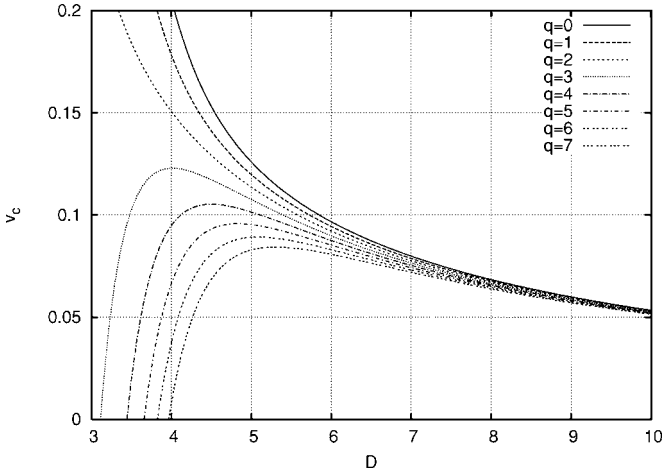


FIG. 6. Plots of Eq. (12) (using all available terms, cf. text) for different values of q.

$$\chi(p) = A(p_c - p)^{-\gamma}[1 + a_1(p_c - p)^{\Delta_1} + \cdots] \tag{16}$$

for $D \neq 6$ and

$$\chi(p) = A(p_c - p)^{-\gamma}|\ln(p_c - p)|^{\delta} + \cdots \tag{17}$$

at the upper critical dimension $D=6$ with $\gamma=1$ and $\delta=2/7$. For $D>6$, one expects a Gaussian fixed point with $\gamma=1$.

We analyse the series using Dlog-Padé approximants, inhomogeneous differential approximants, and the methods termed $M1$ and $M2$ from Refs. [5,33] especially tailored to take confluent nonanalytic correction terms into account. The method $M1$ uses Dlog-Padé approximants to

$$F(p) = (p_c - p)\frac{d\chi}{dp} - \gamma\chi(p), \tag{18}$$

which has a pole at p_c with residue $\Delta_1 - \gamma$. For a given trial value of p_c, the graphs of Δ_1 vs input γ are plotted for different Padé approximants and by adjusting p_c, a point of optimal convergence is searched.

The $M2$ method starts with a transformation of the series in p into a series in $y = 1 - (1 - p/p_c)^{\Delta_1}$, and then Padé approximants to

$$G(y) = \Delta_1(1 - y)\frac{d}{dy}\ln F(y) \tag{19}$$

are calculated, which should converge to γ as $y \to 1$, i.e., $p \to p_c$. These methods are especially useful when taken as biased approximants with a given value of γ or Δ_1 as input. Our results are compiled in Table I, where we also quote for comparison previous estimates based on Monte Carlo simulations and analyses of shorter series expansions.

Generally the series analysis appears to be more difficult for lower dimensions. The p_c we quote for $D=3$ is an average over a large number (ca. 200) of Padé and IDA approximants. The general pattern in the scatter of data is that larger values of p_c corresponds with larger values of the critical exponent γ. The value for γ we quote as our result in three dimensions is obtained by biasing the $M1$ and $M2$ analyses with the more precise p_c value from Monte Carlo simulations. Moving on to $D=4$ and $D=5$ dimensions, nothing spectacular happens and in particular we do not observe any indication of logarithmic corrections to the critical behavior in $D=5$, in accordance with renormalization group expectations and also with newer simulations, cf. the careful discussion of five-dimensional percolation in Ref. [34].

Due to the theoretically expected multiplicative logarithmic corrections (17) at the upper critical dimension a special treatment of the case $D=6$ is needed. The analysis of logarithmic corrections of the general form

$$f(p) \sim (p_c - p)^{-\gamma}|\ln(p_c - p)|^{\delta} \tag{20}$$

is possible [35] by calculating approximants for

$$F(p) = (p_c - p)\ln(p_c - p)\left[\frac{f'(p)}{f(p)} - \frac{\gamma}{p_c - p}\right], \tag{21}$$

where one expects for singularities of the form (20) that $\lim_{p \to p_c} F(p) = \delta$. Using this method biased to $\gamma=1$ we find the values for p_c and δ listed in Table I.

B. The percolation threshold in large dimensions

In Ref. [31], Grassberger compared his Monte Carlo results for p_c with a large-D expansion up to order 5 in $1/D$ [21]. Since we extended this expansion up to order nine, a new comparison may be in order. This expansion is believed to be only asymptotic. Therefore we stop summing up terms of the expansion if the next term is larger than the current one. This recipe results in using only the terms up to order seven in $D=5$ and using all available terms for $D>5$. We also analyzed our susceptibility series at fixed D using differential approximants and the $M1$ and $M2$ methods. Above the critical dimension, the $M1$ and $M2$ methods are used in a variant biased to $\gamma=1$. Our results are collected in Table II.

For higher dimensions our large-dimensionality expansion is in perfect agreement with Grassberger's recent Monte Carlo (MC) data [31], whereas direct analyses of the suscep-

TABLE I. Percolation thresholds (bond percolation on $\mathbb{Z}^D$) and critical exponents. MC is Monte Carlo; MCS is Monte Carlo, **site** percolation; RG is renormalization group; HTS is high-temperature series analysis. References are in square brackets.

D	Methods	p_c	σ	τ	$\gamma=\frac{3-\tau}{\sigma}$
2	exact, CFT	$\frac{1}{2}$	$\frac{36}{91}$	$\frac{187}{91}$	$\frac{43}{18}$
3	MC [25]	0.248 812(2)	0.453(1)	2.189(1)	1.795(5)
	HTS [5]	0.248 8(2)			1.805(20)
	MC [26]	0.248 812 6(5)			
	MCS [27]		0.4522(8)	2.18906(6)	1.7933(85)
	MCS [28]		0.4539(3)	2.18925(5)	1.7862(30)
	present work	0.248 91(10)			1.804(5)
4	HTS [5]	0.160 05(15)			1.435(15)
	MCS [29]				1.44(2)
	MC [30]	0.160 130(3)		2.313(3)	
	MC [31]	0.160 131 4(13)			
	present work	0.160 08(10)			1.435(5)
5	HTS [5]	0.118 19(4)			1.185(5)
	MC [30]	0.118 174(4)		2.412(4)	
	MC [31]	0.118 172(1)			
	present work	0.118 170(5)			1.178(2)
6	RG [32]		$\frac{1}{2}$	$\frac{5}{2}$	$\chi\sim t^{-1}\lvert\ln t\rvert^{\delta}, \delta=\frac{2}{7}$
	HTS [5]	0.094 20(10)			
	MC [31]	0.094 201 9(6)			
	present work	0.094 202 0(10)			$\delta=0.40(2)$
>6	RG		$\frac{1}{2}$	$\frac{5}{2}$	1

tibility series in the respective dimension give slightly larger estimates for p_c. An obvious outlier is $D=6$ where the cutoff criterion for the $1/D$ expansion apparently does not work (taking artificially one term less would significantly improve the estimate).

C. Mean cluster number and moments of the cluster number

Our series for the free energy $\ln Z$ do not allow a reliable estimation of the critical exponent α. This phenomenon is already known from, e.g., Ising model series. One needs higher derivatives $\partial^n \ln Z/\partial p^n$ in order to see a singular contribution which shortens the series, and due to the nature of the nonsingular background, the usual extrapolation methods give much worse results than, e.g., for the susceptibility series.

On the other hand, we can determine some interesting nonuniversal quantities such as the mean number of clusters per site,

$$\langle n_c\rangle = \lim_{\|G\|\to\infty} \langle N_c\rangle/\|G\|, \tag{22}$$

and its nth moments. Here, $\|G\|$ is the number of sites of the graph G. Using $w=q\frac{p}{1-p}$ and denoting the number of edges of the graph by $|G|$, we rewrite the partition sum (2) as

$$Z_G(q,p) = \frac{1}{(1-p)^{|G|}} \sum_C q^{N_c(C)+|C|} p^{|C|} (1-p)^{|G|-|C|}, \tag{23}$$

implying that

$$\langle (N_c+|C|)^n\rangle = \lim_{q\to 1} \frac{1}{Z}\left(q\frac{\partial}{\partial q}\right)^n Z. \tag{24}$$

The mean number of active bonds per side $n_b=|C|/\|G\|$ is for a D-dimensional hypercubic lattice given by $\langle n_b\rangle=pD$, and we obtain

TABLE II. Bond percolation thresholds for hypercubic lattices $\mathbb{Z}^D$ for dimensions $D \geq 5$.

D	Present HT series	MC [31]	Present $1/D$-expansion Eq. (12)
5	0.118 170(5)	0.118 172(1)	0.118 149
6	0.094 202 0(10)	0.094 201 9(6)	0.094 354 3
7	0.078 682(2)	0.078 675 2(3)	0.078 688 1
8	0.067 712(1)	0.067 708 39(7)	0.067 708 0
9	0.059 497(1)	0.059 496 01(5)	0.059 495 1
10	0.053 093 5(5)	0.053 092 58(4)	0.053 092 13
11	0.047 950 3(1)	0.047 949 69(1)	0.047 949 47
12	0.043 724 1(1)	0.043 723 86(1)	0.043 723 76
13	0.040 187 7(1)	0.040 187 62(1)	0.040 187 57
14	0.037 183 8(1)		0.037 183 68

$$\langle n_c \rangle = \lim_{q \to 1} \frac{\partial f}{\partial q} - pD \tag{25}$$

and

$$||G||[\langle (n_c + n_b)^2 \rangle - \langle n_c + n_b \rangle^2] = \lim_{q \to 1} \frac{\partial}{\partial q} \left(q \frac{\partial f}{\partial q} \right), \tag{26}$$

where f is the free energy $\ln Z$ per site.

By using Padé extrapolation to estimate $\partial f / \partial q$ and $\partial^2 f / \partial q^2$ at the percolation threshold p_c, we obtain the estimates for the mean cluster numbers and the variances, Eqs (25) and (26), given in Table III. As usual, the error estimates in Table III characterize the scatter of Padé approximants and do not include systematic errors which are presumably much larger.

For the first number in Table III, the number of clusters per site $\langle n_c \rangle$ in critical $D=2$ bond percolation, Temperley and Lieb derived an exact expression in 1971. This expression was simplified in Ref. [36] to $\langle n_c \rangle = \frac{3\sqrt{3}-5}{2} \approx 0.098\,076$ which affirms our analysis. For bond percolation in three dimensions, Monte Carlo simulations [37] obtained $\langle n_c \rangle = 0.272\,931\,0(5)$. The fluctuations were studied in a recent Monte Carlo simulation [38]. Their results given for $||G||[\langle n_c^2 \rangle - \langle n_c \rangle^2]$ and $||G||[\langle n_c n_b \rangle - \langle n_c \rangle \langle n_b \rangle]$ together with $||G||[\langle n_b^2 \rangle - \langle n_b \rangle^2] = \frac{z}{2} p(1-p)$, where $z=2D$ is the coordination number of the lattice and p equals p_c, imply $||G||[\langle (n_c+n_b)^2 \rangle - \langle n_c+n_b \rangle^2] = 0.164\,45(8)$ for two dimensions and 0.030 71(45) for three dimensions, slightly larger but still consistent with our data.

TABLE III. Mean cluster number and fluctuation.

Dim.	$\langle n_c \rangle$	$\|\|G\|\|[\langle (n_c+n_b)^2 \rangle - \langle n_c+n_b \rangle^2]$
2	0.097 9(1)	0.161(3)
3	0.272 89(3)	0.029 7(5)
4	0.365 494(2)	0.007 56(2)
5	0.411 852(5)	0.003 04(3)
6	0.436 327(5)	0.001 64(1)

VIII. SUMMARY

We successfully applied the method of high-temperature series expansion to q-state Potts model on hypercubic lattices. Modern computer facilities enable the calculation of such series while keeping some parameters (like q or even D) symbolic. This allows one to scan a whole parameter range. Even for the special case $q=1$ we extended the known series by several terms and the results of the singularity analysis are comparable to and in good agreement with Monte Carlo data. By reverting the inverse susceptibility series, we derived the large-D expansion for the (pseudo-)transition point of general q-state Potts models up to order D^{-9}. Further applications, such as the study of the tree percolation limit $q \to 0$, are conceivable, too.

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