Series expansion method based on the droplet description of ferromagnetic and fully frustrated q-state Potts models

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We develop an alternative formalism, based upon the droplet description of critical point phenomena, for calculating the high-temperature (low-density) series expansions for (i) ferromagnetic and (ii) fully frustrated q-state Potts models. For both (i) and (ii), we apply this formalism to explicitly calculate, for the square lattice, the first 20 terms in the series expansion of the general-q partition function. We then obtain from the partition function the series for the mean number of clusters and the specific heat, and analyze the series using Padé approximants. For case (i), the ferromagnetic Potts model, we verify the existence of a geometric transition at the same temperature as the well-known ferromagnetic transition temperature for all q. For case (ii), the fully frustrated Potts model, our analysis reveals the presence of a geometric (percolation) transition at a finite temperature $T_{\rm perc}(q)$, which is well above the critical temperature $T_c = 0$ for these models, but somewhat below the corresponding ferromagnetic transition temperature.

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I. INTRODUCTION

Properties of connectivity transitions in frustrated systems have recently been of much interest [1–8]. The generalization of the droplet formalism to a larger class of systems that includes frustrated systems is an appealing idea with many potential applications, such as the development of a cluster dynamics for frustrated systems [3] analogous to Swendsen-Wang dynamics [4] that could reduce critical slowing down substantially. In particular it has been shown that the cluster formalism of the q-state frustrated Potts model in the limit $q = 1$ leads to a model of frustrated percolation [1,5] that contains as essential ingredients both frustration and percolation; this model can therefore be applied to systems such as spin glasses, glasses, and gels where both connectivity and frustration concepts are important.

The droplet approach to thermal transitions enables one to describe fluctuations in purely geometric terms in terms of critical *droplets*. In the droplet formalism, the partition function of the q-state Potts model is expressed in terms of the bond occupation probability p_B and the number of clusters $N(C)$. Consequently, one can describe thermodynamic transitions in terms of singularities in purely geometric quantities that are traditionally used to describe the percolation transition. In particular, this formulation for general q enables one to calculate the mean number of clusters $\langle N(C)\rangle$ by differentiating the free energy with respect to q. The critical behavior of $\langle N(C)\rangle$ is thus described by the specific heat exponent α.

Straley [9] applied the finite-lattice method [10] to the calculation of the series for tree percolation, which is the $q \to 0$ limit of the q-state Potts model. In this paper, we develop a formalism—based upon the droplet approach—that enables one to calculate the terms in the high-temperature (low-density) series expansion of the partition function of both the ferromagnetic (FM) and fully frustrated (FF) [6] q-state Potts models for general q using the droplet approach [1,7,8]. We first use the droplet approach to extend Straley's method to the case of the FM Potts model for general q and then generalize further to the case of frustrated Potts models. We choose the FF models rather than those with random frustration because our method for calculating the series for the FM models is very easily generalized to the FF case.

We also apply the formalism to explicitly calculate for the square lattice the first 20 terms for both the FM and FF q-state Potts models, keeping q as a free parameter. The series for the FM case yields as special cases random bond percolation ($q \to 1$) [8] and the FM Ising model ($q = 2$), while the series for the FF case yields fully frustrated percolation [1] and the fully frustrated Ising model as special cases. Our results also reduce to tree percolation for $q \to 0$ and agree with the 16 terms calculated by Straley using the finite-lattice method [9], while yielding the next four terms.

II. DROPLET FORMALISM

We begin by briefly reviewing the droplet formalism for the Potts models.

A. Droplet approach to the q-state ferromagnetic Potts models

For the case of the FM Ising model ($q = 2$), the simplest definition of clusters as containing all nearest neighbor (NN) parallel spins is not satisfactory for describing the correlations. In particular, as $T \to \infty$ the range of the correlations should approach zero, but clusters of a finite size still exist due to purely geometrical effects. The droplet model [7] resolves this problem by defining

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a kind of cluster, the *droplet*, which does satisfactorily describe the correlations. These droplets are constructed for the NN FM q-state Potts model by placing bonds between NN parallel spins with a temperature-dependent probability

$$p_B \equiv 1 - e^{-q\beta J}, \tag{1}$$

where $\beta \equiv 1/kT$, k is the Boltzmann constant, and T is the temperature. We may then write the partition function of the N-particle system [1,11] as

$$Z_N = \sum_C \sum_{\{S_i\}} p_B^{|C|}(1-p_B)^{|B|} e^{-\beta \mathcal{H}\{\zeta_i\}}. \tag{2}$$

The NN Potts Hamiltonian is given by

$$\mathcal{H} \equiv -q \sum_{\langle ij \rangle} J_{ij}(\delta_{\zeta_i \zeta_j} - 1) \tag{3}$$

in terms of the Potts variables ζ_i on the N sites i of a lattice. Each ζ_i can take one of the q values and the interactions $J_{ij} = J$ for all NN pairs $\langle ij \rangle$ for the FM case. The sums in (2) are to be carried out over all bond configurations C and all spin configurations such that one is compatible with the other. Here $\mid C \mid$ denotes the number of bonds in configuration C, while $\mid B \mid$ is the number of absent bonds between NN parallel spins. After carrying out the sum over spin configurations [12], we obtain the Fortuin-Kasteleyn [9] expression

$$Z_N(q) = \sum_C p_B^{|C|}(1-p_B)^{|A|} q^{N(C)}. \tag{4}$$

Here $\mid A \mid$ is the total number of absent bonds, $q = 2$ for the Ising case, and $N(C)$ is the number of clusters in configuration C.

Equation (4) defines the alternative description of the model in terms of the purely geometric droplets. These droplets are composed of all NN parallel spins (or in general, Potts variables) that are connected by bonds present with probability p_B given by (1) and are thus subsets of the full clusters. These droplets show percolationlike critical properties at the Potts critical points and thus represent regions of correlated spins. The Potts transition can be viewed from a purely geometric point of view using (4) and, moreover, the formulation for general q enables analysis in terms of geometric percolation quantities such as the mean cluster size (see [11]) and the mean number of clusters $\langle N(C) \rangle = q \ \partial [\ln Z_N(q)] / \partial q$ whose behavior is governed by the same exponents γ and α that govern that of the susceptibility and free energy, respectively, in the thermodynamic formalism.

We next convert Eq. (4) into the form of a high-temperature series. Since $\mid A \mid + \mid C \mid = 2N$, the total number of bonds, we can write (4) as

$$\begin{aligned} Z_N(q) &= \frac{1}{(\mu+1)^{2N}} \sum_b \mu^b \sum_{N_c} G_b(N_c)\, q^{N_c} \\ &= \frac{1}{(\mu+1)^{2N}} \sum_b A_b(q) \mu^b. \end{aligned} \tag{5}$$

Here $\mu \equiv p_B/(1-p_B) = e^{q\beta J} - 1$ is the high-temperature expansion variable and $G_b(N_c)$ is the number of graphs of b bonds with N_c clusters that can be drawn on the lattice and

$$A_b(q) = \sum_{N_c} G_b(N_c)\, q^{N_c}. \tag{6}$$

Equations (5) and (6) define the high-temperature series in μ that we shall calculate and use to analyze the critical behavior of the various Potts models.

B. Extension of droplet approach to frustrated systems

If we let the interactions J_{ij} in (3) now equal J (ferromagnetic) or $-J$ (antiferromagnetic) randomly or systematically (see Sec. III C), we introduce frustration into the system in the sense that all interactions cannot be satisfied by any configuration of spins. A closed loop of interactions C will be frustrated if $\prod_C J_{ij} < 0$, where the product is over all interactions on the loop C. In this case, the droplets are defined [1] in an analogous manner to that for the FM case; one now places bonds with the same probability p_B between two spins whose orientations satisfy the interaction between them. Then, the analog to Eq. (5) for such a system is

$$\begin{aligned} Z_N^F(q) &= \frac{1}{(\mu+1)^{2N}} \sum_b \mu^b \sum_{N_c} G_b^F(N_c) q^{N_c} \\ &= \frac{1}{(\mu+1)^{2N}} \sum_b A_b^F(q) \mu^b, \end{aligned} \tag{7}$$

where now $G_b^F(N_c)$ is the number of graphs of b bonds and N_c clusters *that do not contain frustrated loops* and $A_b^F(q)$ is the quantity analogous to $A_b(q)$ in Eq. (6), with $G_b(N_c)$ replaced by $G_b^F(N_c)$.

We shall refer to the model defined by the partition function of Eq. (7) as the frustrated Potts model. Although Eq. (7) is, for $q = 2$, the partition function of the Ising spin glass Hamiltonian (3) with $J_{ij} = \pm J$, for general $q \neq 2$, it does not correspond to the Hamiltonian (3) but to the Hamiltonian [5] of a particular dilute Potts model.

For frustrated systems, the droplets represent interfering fluctuations that cancel each other to drastically reduce the spin-spin correlations to a range that is much smaller than the mean droplet size [1]. Thus the droplet size is expected to diverge at a temperature $T_{\rm perc}$ that is higher than the spin-glass transition temperature $T_{\rm SG}$ [2]. This temperature $T_{\rm perc}$ thus marks the geometric (percolation) transition for frustrated systems. In two dimensions, we know that $T_{\rm SG} = 0$, but we can expect to find a finite temperature geometric transition at $T_{\rm perc} > 0$.

We shall restrict ourselves here to a specific type of frustrated system, the *fully frustrated* Potts model, which will be defined in Sec. III C.

III. MODELS

First we describe tree percolation, since for this case we can make connection with the 16-term series of Straley

[9]. Then we describe the general-q models for both the FM and FF cases.

A. Tree percolation ($q \to 0$)

To evaluate the series (5) in the limit $q \to 0$ [13], we need to follow a special procedure. First, we rewrite (5)

$$Q_N = \lim_{q\to 0} \frac{Z_N(q)}{q^N} = \lim_{q\to 0} \sum_b (q\beta J)^b \sum_{N_c} G_b(N_c) q^{N_c - N}. \tag{8}$$

However, we know that the number of clusters is given by $N_c = N - b + N_{\rm CL}$, where $N_{\rm CL}$ is the number of closed loops present. Thus, since

$$\lim_{q\to 0} q^{N_{\rm CL}} = \begin{cases} 0 & \text{if } N_{\rm CL} > 0 \\ 1 & \text{if } N_{\rm CL} = 0, \end{cases} \tag{9}$$

only tree configurations (with $N_{\rm CL} = 0$) contribute to the sum in Eq. (8), which can be written as

$$Q_N = \lim_{q\to 0} \sum_b (\beta J)^b \sum_{N_c} G_b(N_c) q^{N_{\rm CL}} = \sum_b T_b z^b, \tag{10}$$

where $z \equiv \beta J$ and T_b is the number of trees (i.e., configurations without any closed loops) of b bonds that can be placed on the lattice. This series (10) was calculated by Straley [9]. Since all closed loops are disallowed in the tree problem, the introduction of frustration makes no difference, and the above expressions remain unchanged.

B. Ferromagnetic q-state Potts model ($q \neq 0$)

For the FM Potts model, the partition function is given by (5). The coefficients T_b in Eq. (10) for the tree series $q = 0$ can be easily obtained from the $A_b(q)$ of Eq. (5); see the last part of Sec. IV for details. For the case $q = 1$, corresponding to random bond percolation, $Z_N(1) = 1$, since Eq. (2) reduces to a binomial expansion of $(p_B + 1 - p_B)^{2N}$. For the case of the Ising model, $q = 2$, the standard definition of the Ising Hamiltonian is slightly different from Eq. (3),

$$\mathcal{H}_I = -J \sum_{\langle ij \rangle} S_i S_j = \mathcal{H} - 2NJ. \tag{11}$$

Thus the partition function Z_N^I corresponding to this Hamiltonian has an extra multiplicative factor of $(\mu+1)^N$ compared to that of Eq. (5):

$$Z_N^I = e^{2\beta JN} Z_N(2) = (\mu + 1)^N Z_N(2). \tag{12}$$

C. Fully frustrated q-state Potts model ($q \neq 0$)

The fully frustrated square lattice (Villain's [6] odd model for the Ising case $q = 2$) is constructed by placing ferromagnetic interactions on all the rows and on alternate columns and antiferromagnetic interactions on the other alternate columns [Fig. 1(a)]. Thus every elementary square (2×2) plaquette on this lattice is frustrated [see Sec. II B and Fig. 1(a)]. However, there are also nonfrustrated closed loops, for example, the 2×3 plaquette, so the allowed configurations consist of more than only tree configurations.

The critical temperature [6] for this fully frustrated model at $q = 2$ is known to be the same as for the Ising spin glass $T_c^{\rm FF} = T_{\rm SG} = 0$, but as for the spin glass, one can expect a percolation transition at a finite temperature for reasons mentioned in Sec. II B. The partition function for this model is given by (7), where the sum marked with an asterisk implies the restriction that any configuration that has all bonds occupied on a frustrated plaquette (such as the 2×2 square) will be omitted from the sum. This type of frustration turns out to be easier to deal with because we do not need to average over different realizations of ferromagnetic and antiferromagnetic interactions, as one would have to do for the case of random frustration. We deal instead with the single fixed realization of alternating interactions described above. Thus the FF series can be obtained from the FM series by subtracting the contribution from configurations containing frustrated closed loops [Fig. 1(c)].

For the FF Ising case, to compare with the known partition function [6], one must once again multiply by $(\mu + 1)^N$ as in (12).

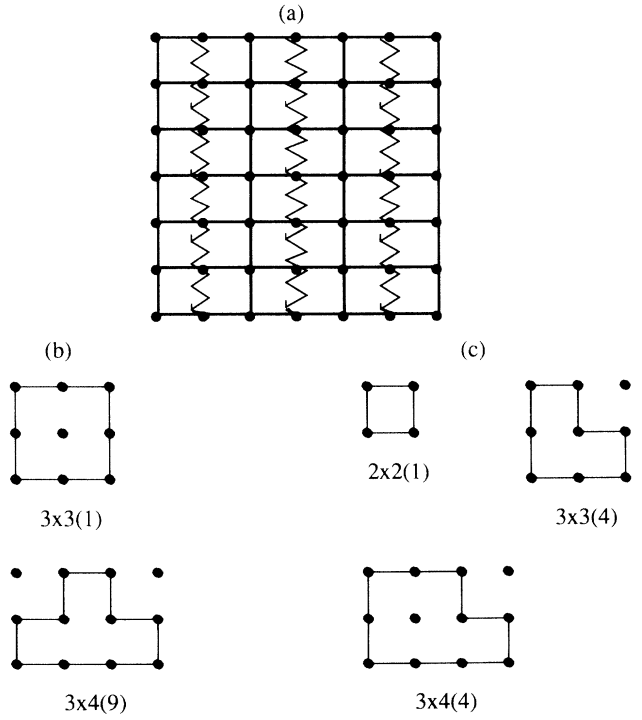

FIG. 1. (a) The fully frustrated square lattice. Straight lines indicate ferromagnetic bonds while wavy lines indicate antiferromagnetic bonds. (b) Examples of nonfrustrated closed loops. The numbers below each loop, $L \times M(C_k^{\rm NF})$, indicate the number $C_k^{\rm NF}$ of nonfrustrated NSG for that value of $L \times M$. (c) The same for frustrated loops, with $L \times M(C_k^F)$ being the numbers below each loop [see Eq. (19)].

IV. METHOD

In this section, we develop a method for calculating the high-temperature series for the partition functions of the FM (5) and FF (7) q-state Potts models within the droplet formalism.

The principal advantage of the method is that to calculate the first k terms in the infinite lattice partition function, we need only evaluate the partition functions of finite lattices up to a perimeter k. Thus we start by evaluating the series Eq. (5) for all finite lattices of perimeter less than or equal to the order of the highest term required in the series expansion. We label the polynomial in μ for the partition function of an $L \times M$ rectangle by $P_{LM}(q)$, following the notation in [9]. More explicitly [see Eq. (5)],

$$P_{LM}(q) = (\mu+1)^{2N} Z_N(q) = \sum_b A_b(q)\mu^b, \tag{13}$$

where $N = L \times M$ = total number of sites and $A_b(q)$ is given by Eq. (6). Then, since the expansion is in powers of μ, with the number of bonds b being the power, the polynomial for the smallest such lattice (a single bond) is $P_{12}(q) = P_{21}(q)$; this is the partition function for two nn sites $P_{12}(q) = q^2 + q\mu$ (see Appendix A and Fig. 3 for details). Now, we construct the *reduced series* $R_{LM}(q)$ for this finite rectangle by dividing $P_{LM}(q)$ by the reduced series of all rectangles enclosed by this $L \times M$ rectangle,

$$R_{LM} = \frac{P_{LM}}{\prod\limits_{L' \times M' \in L \times M} R_{L'M'}}. \tag{14}$$

Now the dependence of all the P_{LM} and the R_{LM} on q is kept implicit. We start by defining the reduced series for the smallest rectangle as $R_{12} \equiv P_{12}$ and then construct the reduced series for all larger rectangles required using the prescription (14) (Fig. 1). Thus, for example, $R_{22} = P_{22}/R_{12}^4$ and $R_{23} = P_{23}/(R_{12}^7 R_{22}^2)$ and so on.

Then, from the definition (14), the partition function $Z_N = P_{LM}$ of any lattice of $N = L \times M$ sites can be written as a product over the reduced series $R_{L'M'}$ of all $L' \times M'$ rectangles enclosed by this $L \times M$ rectangle. In particular, as $N \to \infty$, each rectangle is contained N times and thus in the thermodynamic limit

$$Z_N(q) = \prod_{LM} R_{LM}^N(q). \tag{15}$$

The partition function per site $Z_1 = (Z_N)^{1/N}$ is simply the product of the reduced series for each rectangle taken once. Thus, for example, we have to $O(\mu^{20})$

$$\begin{aligned} Z_1 = {} & R_{12}^2 R_{22} R_{23}^2 R_{33} R_{24}^2 R_{34}^2 R_{25}^2 R_{44} R_{35}^2 R_{26}^2 R_{45}^2 R_{36}^2 \\ & \times R_{27}^2 R_{55} R_{46}^2 R_{37}^2 R_{28}^2 R_{66} R_{57}^2 R_{48}^2 R_{39}^2 R_{2,10}^2, \end{aligned} \tag{16}$$

where all rectangles up to a perimeter of 20 have been included. This is because the reduced series in general has the form

$$R_{LM} = 1 \pm a_k \mu^k + O(\mu^{k+1}), \tag{17}$$

where the leading power $k = 2(L+M) - 4$ is the perimeter of the $L \times M$ rectangle and a_k is a coefficient that depends on the model in question. Therefore, only rectangles of perimeter $\leq k$ contribute to the first k terms in the partition function series and thus only the reduced series for these rectangles need to be evaluated. In particular, for the tree percolation problem, it was found in [9] that the reduced series have the form

$$R_{LM}^T = 1 - c_k z^k + O(z^{k+1}), \tag{18}$$

where c_k is the number of nondecomposable graphs with closed loops that fit into this $L \times M$ rectangle, but not in any smaller one. For future reference we will refer to such graphs as *nondecomposable spanning graphs* (NSG's).

We find that for the general q-state Potts model, the reduced series have the form

$$R_{LM}^P = 1 + \frac{\mu^k}{q^k}\left[(q-1)\,C_k^{\mathrm{NF}} - C_k^F\right] + O\left(\mu^{k+1}\right), \tag{19}$$

where C_k^{NF} is the number of NSG's on the $L \times M$ lattice of perimeter k that are not frustrated and C_k^F is the number that are frustrated. For example (Fig. 1), $C_k^{\mathrm{NF}} = 1$ and $C_k^F = 4$ for the 3×3 rectangle ($k = 8$) for the FF Potts model. The reduced series for the FM Potts case are obtained from Eq. (19) by substituting $C_k^F = 0$. For the Ising model ($q = 2$) we have, from (19),

$$R_{LM} = 1 + \frac{\mu^k}{q^k}\left(C_k^{\mathrm{NF}} - C_k^F\right) + O\left(\mu^{k+1}\right). \tag{20}$$

Expressions (17)–(20) serve as a good check on our calculations of the P_{LM}. Moreover, they enable us to push the series to one higher order than is determined by the calculation of the P_{LM} (see the description of the transfer matrix method at the end of this section for details). For an explicit calculation of the first five terms in the series for the partition function, see Appendix A.

We next proceed to calculate the partition function to higher orders, first for the FM Potts case. To do this, we need the polynomials P_{LM} for lattices of perimeter up to 20, i.e., all $L \times M$ lattices for $L + M \leq 12$. We calculate these by a transfer matrix method [14] that generates $P_{L,M+1}$ from P_{LM} by adding a row of L sites. In order to do this, we start with $P_{L,1}$ in the form of a column vector, with each element of the vector representing the weight of a particular "type" of edge configuration. The information needed to describe a particular type of edge configuration is the connectivity of the L sites on the edge of the lattice, i.e., which sites are connected to each other (for details on the transfer matrix method, see Appendix B). We calculate the transfer matrix for $L = 2$, $L = 3$, $L = 4$, and $L = 5$ thus obtaining all the required polynomials P_{LM} and consequently all the reduced series R_{LM} [from (14)] with $L + M \leq 12$, except for R_{66}. For R_{66}, one would normally need to calculate the transfer matrix for $L = 6$ (a tedious process); however, now we can use Eq. (19) to get

$$R_{66} = 1 + 19010(q-1)\mu^{20}/q^{20} + O(\mu^{21}). \tag{21}$$

Then we use (16) to get the partition function per site

$Z_1(q)$ for the q-state FM Potts model to $O(\mu^{20})$.

For the FF case, we follow a similar procedure as the FM case above, with a few modifications: now the information needed about the sites on the edge of the lattice is more than just their connectedness to other sites. For this frustrated case, we need the additional information about *how* the sites in question are connected. To be more specific, we need to know whether the connection is such that closing the loop at the next application of the transfer matrix will result in a frustrated loop or not. Thus each connection between two of the L edge sites can be of two types and there are many more types of edge configurations. Therefore, the dimension of the transfer matrix for a particular L is considerably higher for the frustrated case than for the FM (for more details on the method, see Appendix B). This gives the finite-lattice polynomials P_{LM}. We then obtain the reduced series from (14) and the partition function $Z_1^F(q)$ from (16) to $O(\mu^{20})$ using the four transfer matrices for $L = 2$, $L = 3$, $L = 4$, and $L = 5$. For R_{66}, we use (19) to get $R_{66} = 1 + (9400q - 19010)\mu^{20}/q^{20} + O(\mu^{21})$, since 9400 of the total number 19010 of NSG's for the 6×6 lattice are not frustrated ($C_{20}^{\mathrm{NF}} = 9400$).

For the FM Potts models, we have $C_k^F = 0$ in (19). In particular, for $q = 1$ (random bond percolation) we find from (19) that $R_{LM} = 1$ for all L and M and thus from (15), $Z_N(1) = 1$ and the free energy $F(q = 1) = -\ln Z_N(1) = 0$, as is expected from Eq. (4) for $q = 1$. The correct generating function for this series (see, for example, [7] and [8]) is

$$G(q) = \left.\frac{dF(q)}{dq}\right|_{q=1} = \lim_{q\to 1} \frac{F(q)}{(q-1)}. \tag{22}$$

We also compared the series we obtain using our prescriptions (3), (14), (20), and (15) for the reduced series and partition function with the standard Ising high-temperature series and verified that it gives the same results, though expanded in a different variable. We also checked the same for the FF Ising case by expanding Villain's exact partition function [6] in a high-temperature series and once again verified our results.

The coefficients $B_b(q) = q^b A_b(q)$ and $B_b^F(q) = q^b A_b^F(q)$ obtained in the series expansion of the partition function for the FM and FF q-state Potts models described in Sec. III are given in Table I. The coefficients T_b in (10) for tree percolation can be obtained from these as follows. The partition function for the tree case is

$$\lim_{q\to 0} \sum_b A_b(q)\mu^b = \sum_b \left[\lim_{q\to 0} B_b(q)\right] z^b, \tag{23}$$

where $z \equiv \beta J$. Comparing with (10), we then get $T_b = \lim_{q\to 0} B_b(q) = \lim_{q\to 0} B_b^F(q)$, since configurations with no closed loops are the same for the frustrated and nonfrustrated cases. These correspond to the tree configurations listed in Table I.

TABLE I. Coefficients in the expansion of the partition function per site $Z_1 = Z_N^{1/N}$.

b	T_b	$q^b A_b(q)$	$q^b A_b^F(q)$
0	1	1	1
1	2	2	2
2	1	1	1
3	0	0	0
4	−1	$(q-1)$	-1
5	2	$-2(q-1)$	2
6	−5	$5(q-1)$	$-(5-2q)$
7	16	$-2(q-1)(8-q)$	$2(8-5q)$
8	−54	$6(q-1)(9-2q)$	$(31q-54)$
9	184	$-2(q-1)(92-27q)$	$8(23-11q)$
10	−628	$2(q-1)(3q^2-114q+314)$	$(2q^2+281q-628)$
11	2136	$-2(q-1)(29q^2-464q+1068)$	$-2(3q^2+508q-1068)$
12	−7229	$(q-1)(q^3+361q^2-3663q+7229)$	$-(61q^2-3790q+7229)$
13	24738	$2(q-1)(4q^3-949q^2+7069q-12189)$	$2(342q^2-6910q+12189)$
14	−82185	$-3(q-1)(60q^3-3058q^2+17933q-27395)$	$3(2q^3-1310q^2+16358q-27395)$
15	278276	$2(q-1)(4q^4+828q^3-21105q^2+101684q-139138)$	$-2(23q^3-8705q^2+86294q-139138)$
16	−951192	$-(q-1)(46q^4+11489q^3-188490q^2+768789q-951192)$	$(92q^3-69828q^2+611834q-951192)$
17	3296080	$2(q-1)(q^5-119q^4+34741q^3-413410q^2+1460277q-1648040)$	$4(50q^3+69785q^2-551916q+824020)$
18	−11601580	$(q-1)(10q^5+5953q^4-387468q^3+3586980q^2-11174965q+11601580)$	$2(13q^4+883q^3-576728q^2+4058696q-5800790)$
19	41444452	$2(q-1)(-92q^5-30542q^4+1022504q^3-7717428q^2+21525977q-20722226)$	$-2(165q^4+24404q^3-2435059q^2+15145719q-20722226)$
20	−149801793	$(q-1)(22q^6-216q^5+474088q^4-10356148q^3+65910515q^2-166629530q+149801793)$	$(1938q^4+452701q^3-20515919q^2+114059417q-149801793)$

V. ANALYSIS

We now calculate from the partition function the series for the specific heat, and for its geometric analog, the temperature derivative of the mean number of clusters per site $\langle N(C)\rangle/N$ given by [from Eq. (4)]

$$\frac{\langle N(C)\rangle}{N} = q\frac{\partial \ln Z_1}{\partial q}. \tag{24}$$

For the case $q = 1$ (random bond percolation), we first evaluate the quantity $G(q)$ in Eq. (22), which plays the role of the free energy for this case, and then form the double derivative to obtain the specific heat series. The analysis of the specific heat and its geometric analog, the first derivative (for $q \neq 1$) or the second derivative (for $q = 1$) of the mean number of clusters, for the various q shows that both functions indeed undergo a transition at the same temperature for all q.

This transition temperature for the FM series agrees very well with previous results [15] on the thermodynamic transition in Potts systems (Fig. 2). The exponent $\alpha(q)$, however, is difficult to obtain accurately from the Padé approximants, and we need more sophisticated methods of analysis.

For the FF Potts series, we obtain transition temperatures $T_{\rm perc}(q)$ (Fig. 2) that are somewhat lower than those for the corresponding FM series (as expected, frustration makes the transition to an ordered state more difficult and thus lowers the transition temperature), but considerably higher than the critical temperature $T = 0$ for these models at $d = 2$. For $q < 2$, the singularities at $T_{\rm perc}$ are extremely weak and do not show up in the Padé analysis of the derivatives of F and $\langle N(C)\rangle$. To analyze the FF series for these low values of q, we follow Straley [9] and calculate the series $\rho(\mu)$ for the average bond density from (7) (note that for frustrated systems, this is different from the probability of a bond being occupied):

$$\rho(\mu) = \frac{\langle b\rangle}{2N} = \frac{\mu}{2N}\frac{\partial \ln Z_N}{\partial \mu} = \frac{\mu}{2Z_1}\frac{\partial Z_1}{\partial \mu}. \tag{25}$$

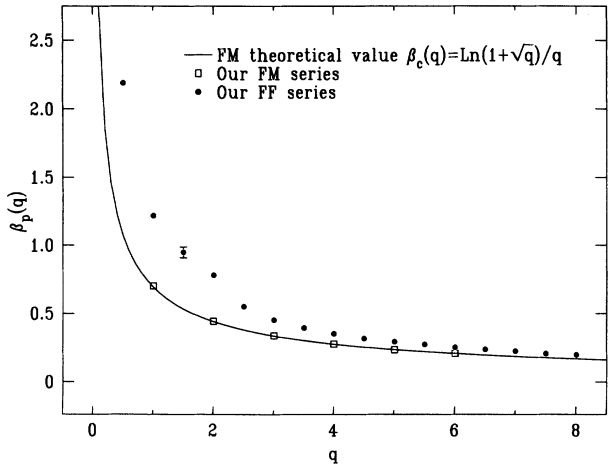

FIG. 2. Inverse transition temperatures $\beta_{\rm perc}(q) = 1/T_{\rm perc}(q)$ vs q for the FM and FF cases. The bold line is the theoretical transition line $\beta_{\rm perc}(q) = \ln(1+\sqrt{q})/q$ for the FM case.

We then invert this series to obtain the series $\mu(\rho)$ and then do a Padé analysis to find the critical bond density ρ^*. For $q = 1$ (fully frustrated percolation), we find $\rho^* \simeq 0.5281$. Since the maximum (close-packing) density for this fully frustrated Potts model is $\rho_{\rm CP} = 0.75$, we can write the approximate relation (exact only at $T = 0$, thus expected to be reasonable at the low temperatures we're dealing with) for the percolation threshold $p_c(q = 1) \simeq \rho^*/\rho_{\rm CP} \simeq 0.704$. We can then calculate the inverse of the connectivity transition temperature $\beta_{\rm perc}(q)$ from

$$p_B = 1 - e^{-q\beta_{\rm perc}J} = p_c(q) \simeq \rho^*(q)/\rho_{\rm CP}, \tag{26}$$

which gives us the points in Fig. 2 for $q = 1/2$, $q = 1$, and $q = 3/2$ for the FF case.

Analysis of the series coefficients T_b for the tree series [9] corresponding to $q = 0$ gives $\rho^*(q = 0) = 0.5$, which is the close-packing density $\rho_{\rm CP}$ for the tree problem. Thus $\beta_{\rm perc}(q = 0) = \infty$ for this case and both the FM and FF curves in Fig. 2 should approach ∞ as $q \to 0$, which seems consistent with our results.

VI. DISCUSSION

We have developed a method for calculating high-temperature series for the q-state Potts model using the droplet formalism and extended it to the case of frustrated systems. We calculated the series for the FM and FF cases. The method can be generalized to incorporate random frustration as well and thus to study spin glasses. For such a generalization, the contribution of frustrated and nonfrustrated configurations of interactions $\{J_{ij}\}$ to each closed loop must be multiplied by the probability $P(\{J_{ij}\})$ for such a configuration.

We believe that this method will be particularly useful for evaluating series for models (such as frustrated models) in which certain graphs with closed loops are systematically forbidden. One of the principal advantages of the present method is that it enables us to evaluate the partition function of the q-state Potts model with q as a free parameter. First, this makes it possible to calculate percolation quantities of interest (such as the mean number of clusters, the connectivity analog of the free energy) and second, enables the immediate evaluation of the partition function for any q, including fractional values.

ACKNOWLEDGMENTS

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APPENDIX A: EXPLICIT CALCULATION OF THE FIRST FIVE TERMS IN THE SERIES FOR THE PARTITION FUNCTION

Here we calculate the first five terms in the partition function as an explicit example. To obtain $Z_1(q)$ to $O(\mu^4)$, we only need to calculate P_{21} and P_{22}, since

we need rectangles up to perimeter 4.

For the FM case, we have [see Fig. 3 and Eq. (13)]

$$P_{21}(q) = q^2 + q\mu \tag{A1}$$

and

$$\begin{aligned} P_{22}(q) &= q^4 + 4q^3\mu + 6q^2\mu^2 + 4q\mu^3 + q\mu^4 \\ &= (\mu + q)^4 + (q-1)\mu^4. \end{aligned} \tag{A2}$$

We know that to this order $Z_1 = R_{21}^2 R_{22}$ [see Eqs. (14) and (16)]. Then, since $R_{21} = P_{21}$ and $R_{22} = P_{22}/R_{21}^4$, we have

$$Z_1(q) = P_{22}/P_{21}^2 = \left[(\mu+q)^4 + (q-1)\mu^4\right]/(q^2+q\mu)^2. \tag{A3}$$

This, when expanded to $O(\mu^4)$, gives

$$Z_1(q) = 1 + 2\mu/q + \mu^2/q^2 + (q-1)\mu^4/q^4, \tag{A4}$$

which are the first five entries in the third column of Table I. We can obtain the standard Ising series from this by substituting $q = 2$ and $\mu = \exp(2K) - 1$ and dividing by $(\mu + 1)$ [see Eq. (12)]; this gives

$$Z_1^I = 1 + K^2 + 4K^4/3, \tag{A5}$$

where $K \equiv \beta J$.

Now, for the FF case, P_{21} is the same as the FM case (A1), since no closed loops are involved. For P_{22}^F, the last configuration in Fig. 3 does not contribute, since one cannot occupy all four bonds on the 2×2 square without creating a frustrated loop. Thus

$$P_{22}^F(q) = q^4 + 4q^3\mu + 6q^2\mu^2 + 4q\mu^3 = (\mu+q)^4 - \mu^4. \tag{A6}$$

Again,

$$Z_1^F = P_{22}^F/P_{21}^4 = \left[(\mu+q)^4 - \mu^4\right]/(q^2+q\mu)^2 \tag{A7}$$

and expanding this out gives the first five entries in the fourth column of Table I:

$$Z_1(q) = 1 + 2\mu/q + \mu^2/q^2 - \mu^4/q^4, \tag{A8}$$

which, on making the same substitutions as for (A5), gives for the standard FF Ising series:

$$Z_1^{\mathrm{FFI}} = 1 + K^2 - 2K^4/3. \tag{A9}$$

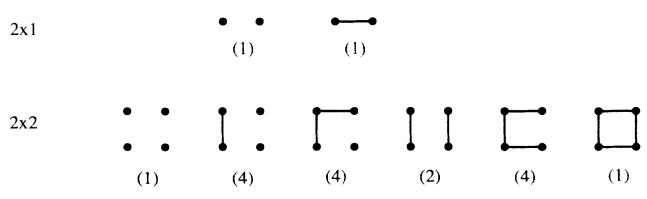

FIG. 3. Configurations contributing to P_{LM} (for $L \times M$ equal to 2×1 and 2×2) with their degeneracies in brackets below each configuration.

APPENDIX B: TRANSFER MATRIX

Each application of the transfer matrix adds a horizontal layer of L sites to the lattice and transforms one type of configuration of L sites at the edge [classified in terms of their connectivity to other sites at the edge; see Fig. 4(a)] to another, while adding a new row of sites. The dimensionality of the transfer matrix is equal to the number of such unique edge configurations. For the FM case then, this is 2, 4, 10, and 26 for $L = 2$, 3, 4, and 5, respectively. See Fig. 4(a) for an explicit illustration of edge configurations for $L = 2$ and $L = 3$. For $L = 2$, the lowest polynomial corresponds to the partition function for a single pair of adjacent spins $P_{21} = q^2 + q\mu$ [from Eq. (13)], where the two terms represent the two configurations in Fig. 3(a). We represent this by the vector $M_{21} = (q^2, q\mu)$. The transfer matrix is applied in two stages. First, one adds the L vertical bonds: this operation is represented by the matrix V_L. An occupied bond is associated with a factor μ [the number of clusters $N(C)$ remains unchanged] and a vacant one with a factor q [$N(C)$ increases by one]. For example, for $L = 2$ we have

$$V_2 = \begin{pmatrix} \mu^2 & 0 \\ 2\mu q + q^2 & \mu^2 + 2\mu q + q^2 \end{pmatrix}. \tag{B1}$$

The second stage consists of adding the $(L-1)$ horizontal bonds and is represented by a matrix H_L. Now, we associate a factor μ with an occupied bond between previously connected sites, a factor μ/q [since $N(C)$ decreases by one] with an occupied bond between previously unconnected sites and a factor 1 for a vacant bond. Again, for $L = 2$,

$$H_2 = \begin{pmatrix} 1+\mu & \mu/q \\ 0 & 1 \end{pmatrix}. \tag{B2}$$

The full transfer matrix is then given by $T_L = H_L V_L$. The operation of adding a row of L sites is represented by $M_{LM} = T_L M_{L,M-1}$ with the corresponding polynomial P_{LM} being the sum of elements of M_{LM}.

For the frustrated case, the number of edge configurations and thus the dimensionality of the transfer matrix is higher than the FM case at 3, 8, 30, and 112 for $L =$ 2, 3, 4, and 5, respectively [see Fig. 4(b)]. This is be-

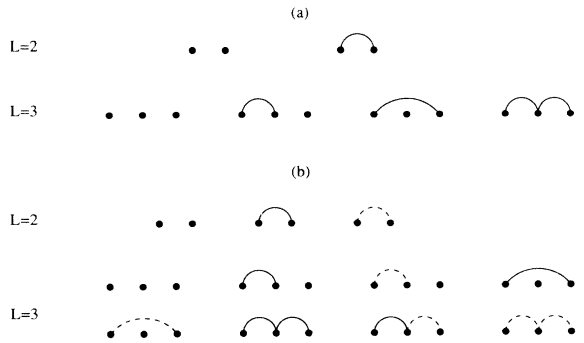

FIG. 4. Edge configurations for the transfer matrix for the (a) FM case and (b) FF case.

cause each category of configurations of sites on the edge for the FM case corresponds to one or more for the frustrated case, since each connection between two sites in the FM case can now be of two types [see Fig. 4(b) for an explicit illustration for $L = 2$ and $L = 3$]: one that will lead to a frustrated loop on being closed at the next application of the transfer matrix (indicated by a dashed line) and one that will not (indicated by a solid line). For this case, the lowest polynomial $P_{21}^F = P_{21}$ (since there are no closed loops) with $M_{21}^F = (q^2, 0, q\mu)$ corresponding to the three configurations of Fig. 4(b). The first stage of the application is the same as the FM case, except for the dimensionality of the transfer matrix being higher. For $L = 2$, this is represented by

$$V_2^F = \begin{pmatrix} \mu^2 & 0 & 0 \\ 0 & \mu^2 & 0 \\ 2\mu q + q^2 & 2\mu q + q^2 & (\mu + q)^2 \end{pmatrix}. \tag{B3}$$

The second stage is slightly different, since the addition of a horizontal bond can lead to the closure of a frustrated loop. Thus, in terms of the factors associated with each bond, the difference from the FM case above is that we now have a factor μ for an occupied bond between previously connected sites *that does not close a frustrated loop* and a factor 0 for one that does. Again we have for $L = 2$

$$H_2^F = \begin{pmatrix} 0 & 1 & 0 \\ 1+\mu & 0 & \mu/q \\ 0 & 0 & 1 \end{pmatrix}, \tag{B4}$$

and, as before, the full transfer matrix is $T_L^F = H_L^F V_L^F$ with $M_{LM}^F = T_L^F M_{L,M-1}^F$ and P_{LM}^F being the sum of the elements of M_{LM}^F. The matrices V_L and H_L for higher L are given in [12].

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