Geometry, thermodynamics, and finite-size corrections in the critical Potts model

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(Received 22 January 1999; revised manuscript received 6 July 1999)

We establish an intriguing connection between geometry and thermodynamics in the critical q-state Potts model on two-dimensional lattices, using the q-state bond-correlated percolation model (QBCPM) representation. We find that the number of clusters $\langle N_c \rangle$ of the QBCPM has an energylike singularity for $q \neq 1$, which is reached and supported by exact results, numerical simulation, and scaling arguments. We also establish that the finite-size correction to the number of bonds, $\langle N_b \rangle$, has no constant term and explains the divergence of related quantities as $q \to 4$, the multicritical point. Similar analyses are applicable to a variety of other systems. [S1063-651X(99)09612-9]

PACS number(s): 05.50.+q, 64.60.Fr, 75.10.−b

Percolation [1] and the q-state Potts model (QPM) [2] are related to many interesting problems in mathematics and science and are ideal models for studying critical phenomena [1–8]. In recent years, much attention has been paid to universal quantities at or near the percolation point, such as the critical existence probability E_p or crossing probability [4], finite-size scaling functions [5], excess cluster numbers [6,7], etc. In a recent paper, Ziff *et al.* [6] calculated the number of clusters per lattice site n in percolation on two-dimensional lattices with N lattice sites and periodic boundary conditions (PBC). They found that $n = n_c + b/N + \cdots$, where n_c is n in the limit $N \to \infty$ and b is a positive universal constant that may be calculated using conformal field theory (CFT) [7]. In this paper, we consider the q-state bond-correlated percolation model (QBCPM) [9] on planar lattices G of N sites and E bonds, which is equivalent to the QPM on G; the numbers of bonds and clusters of a subgraph G' of G are denoted by $N_b(G')$ and $N_c(G')$, respectively. In the QBCPM, as in ordinary percolation, a natural focus on geometric properties such as cluster number arises. However, the system also has nontrivial thermodynamics, impelling an investigation of the connections between geometry and thermal behavior. In this work we concentrate on the critical Potts models for definiteness; however, our methods are much more generally applicable, as pointed out below.

We address this question by investigating the universal behavior of finite-size corrections (FSC). We show by exact calculation that when $q \neq 1$, the FSC for $\langle N_c \rangle$ is linearly related to the FSC for $\langle N_b \rangle$, i.e., surprisingly, the number of clusters has an energylike singularity. This is quite different from the case $q = 1$, which is equivalent to bond random percolation [10] studied by Ziff *et al.* [6,7]. Numerical simulation, scaling theory for the infinite system, and finite-size scaling arguments verify and illuminate this conclusion. The latter also implies that $\langle N_b \rangle$ has no constant finite-size scaling term at criticality, which we verify explicitly for the Ising model on a square lattice. We also find that the FSC of $\langle N_c + g N_b \rangle$ and its higher cumulants (where g is defined below, and $g = 1/2$ for a square lattice) diverge as $q \to 4$, which is attributable to the onset of logarithmic corrections at the multicritical point and is understandable from a renormalization-group (RG) picture.

Here we briefly review the connection between the QPM and the QBCPM [9,11]. In the QPM, each site of the lattice G is occupied by a spin s_i with spin components $-s, -s+1, \ldots, s-1$, and s, where $1 \leqslant i \leqslant N$, $2s+1 = q$, and q is an integer. The Hamiltonian of the QPM is given by

$$-H/k_B T = K \sum_{\langle i,j \rangle} \delta(s_i, s_j) + B \sum_i s_i . \tag{1}$$

Here the first summation is a sum over all nearest neighbors, $\delta(s_i, s_j) = 1$ or 0 when $s_i = s_j$ or $s_i \neq s_j$, respectively, $K = J/k_B T > 0$ is the normalized NN coupling constant, and $B = h/k_B T$ is the normalized external magnetic field with k_B being the Boltzmann constant and T being the absolute temperature.

Using the subgraph expansion of Eq. (1), Hu has shown that phase transitions of the QPM are percolation transitions of the QBCPM, in which a subgraph G' appears with the weight

$$\pi(G', p, q) = p^{N_b(G')} (1-p)^{E - N_b(G')} q^{N_c(G')}, \tag{2}$$

where $p = 1 - \exp(-K)$; the spontaneous magnetization M and the magnetic susceptibility χ of the QPM are related to the percolation probability P and the mean cluster size S of the QBCPM, respectively. These connections ensure that phase transitions of the QPM are percolation transitions of the QBCPM [9]. The partition function of the QPM at zero magnetic field may be written as

$$Z_N = \sum_{G'} [\exp(K) - 1]^{N_b(G')} q^{N_c(G')}$$

$$= \exp(KE) \sum_{G'} \pi(G', p, q). \tag{3}$$

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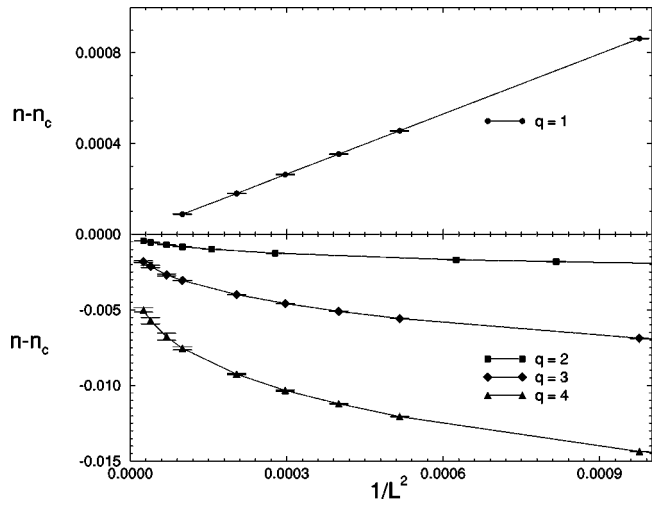

FIG. 1. $n-n_c$ as a function of $1/L^2$ for the QBCPM on $L\times L$ square lattices with PBC (torus) for $q=1$, 2, 3, and 4.

Here the sum is over all G' of G [10]. The internal energy U and the specific heat C_h of the QPM are related to the average number of occupied bonds $\overline{p}$ and the fluctuations of the number of occupied bonds C_{2b} of the QBCPM, respectively [9].

Using the Swendsen-Wang algorithm [12], we calculate the average number of clusters per site n of the critical QBCPM on $L'\times L$ square lattices with PBC in both horizontal and vertical directions; the number of spin components q is an input parameter taken to be 1, 2, 3, and 4. It should be noted that n in the limit L', $L\to\infty$, denoted by n_c, follows from exact results for the critical Potts free energy on several planar lattices [2,13]. We plot $n-n_c$ as a function of $1/L^2$ in Fig. 1 which shows that the data for $q=1$ are on a linear curve. The linear least-square fit of these data gives $n_c=0.09807(6)$ and the slope $b=0.884\pm0.002$, which are consistent with the result of Ziff *et al.* [6,7]. However, results for $q=2$, 3, and 4 are quite different, namely the curves for $q\geqslant 2$ have negative slopes, which suggests that the argument of Ziff *et al.* [6] to relate the slope b to the average number of clusters wrapping around the toroidal system is invalid and signals a new behavior as we show below.

To understand the curves in Fig. 1 for $q\geqslant 2$, consider the partition function Z_c of the planar lattice QPM at the critical point $p_c=1-e^{-K_c}$:

$$Z_c=\sum_{G'}[f(q)]^{N_b(G')}q^{N_c(G')}. \tag{4}$$

Here $f(q)=e^{K_c}-1$ and is known exactly for square, planar triangular, and honeycomb lattices [2]; for a square lattice, $f(q)=\sqrt{q}$. Z_c is supposed to factor as $Z_c=Z_nZ_u$, where Z_n is a nonuniversal factor and the universal factor Z_u gives FSC. Exact results for Z_u follow from the Coulomb gas formulas of Di Francesco, Saleur, and Zuber (DFSZ) [14]. The cumulants C_n of N_c+gN_b are given by $C_n=[q(\partial/\partial q)]^n\ln Z_c$, where $g=g(q)=qf'(q)/f(q)$ and is 1/2 for the square lattice. Since $Z_u=Z_u(L'/L)$, FSC's to C_n are scale invariant. Thus, as in [7] for $q=1$

$$C_n=a_nLL'+b_n(L'/L)+O(1/L), \tag{5}$$

where b_n is the universal FSC and may be derived from DFSZ [14]. It follows that there is no divergent FSC term for any C_n for $q<4$. In particular, for $n=1$ we have

$$C_1=\langle N_c+gN_b\rangle=a_1LL'+b(L'/L)+O(1/L). \tag{6}$$

For $q=2$, $b(1)=0.967\,734\ldots$ and $b(2)=1.064\,63\ldots$; for $q=3$, $b(1)=1.057\,79\ldots$ and $b(2)=1.133\,21\ldots$. Since $\langle N_b\rangle$ is proportional to the internal energy, which has a singular FSC proportional to $L^{1/\nu}$ at criticality, Eq. (6) implies that the FSC for $\langle N_c\rangle$ has an energylike singularity with amplitude $-g$ times the amplitude of $\langle N_b\rangle$. A similar argument holds for any C_n, suggesting that $N_c\approx -gN_b$ in the sense of FSC, i.e., we can replace N_c by $-gN_b$ to calculate any leading FSC.

This conclusion also follows from scaling for the infinite system. The singular part of the free energy per site f_s may be written as $f_s\approx A(q)[p-p_c(q)]^{2-\alpha(q)}$, where $A(1)=0$ for (random) percolation and α is the specific heat exponent. Differentiating f_s with respect to q, we find $\langle N_c\rangle\approx -A(q)p_c'(q)[p-p_c(q)]^{1-\alpha(q)}LL'$, showing that $\langle N_c\rangle$ is energylike to leading order for $q\neq 1$.

The universal (singular) part of the free energy F_u is defined above at the critical point. According to finite-size scaling theory [15], F_u also extends to large but finite systems near criticality, with

$$F_u=LL'f_u\approx\psi[(\beta-\beta_c)L^{1/\nu}]LL'$$

$$\approx B+(\beta-\beta_c)CL^{1/\nu}-\frac{1}{2}(\beta-\beta_c)^2DL^{2/\nu}+\cdots. \tag{7}$$

Here β_c, ν, B, C, and D depend on q; B, $CL^{1/\nu}$, and $DL^{2/\nu}$ determine the universal (singular) terms in the free energy, internal energy, and specific heat at the critical point, respectively. Let $x=e^{\beta J}-1$, then $x_c=f(q)$. Using the total partition function Z_N and $\langle N_c\rangle=q(\partial/\partial q)\ln Z_N$, $\langle N_b\rangle=(\partial/\partial x)\ln Z_N$, we find for $\beta=\beta_c$ that

$$\langle N_c(G')\rangle\approx n_cLL'-\frac{qf'(q)}{J(x_c+1)}CL^{1/\nu}+qB'(q), \tag{8}$$

$$\langle N_b(G')\rangle\approx n_bLL'+\frac{f(q)}{J(x_c+1)}CL^{1/\nu}. \tag{9}$$

Note that exact results for n_b are available and $n_b=1$ for the square lattice Potts model for any q [2]. Therefore,

$$C_1=\langle N_c+gN_b\rangle=a_1LL'+qB'(q), \tag{10}$$

where $a_1=n_c+gn_b$, which agrees with Eq. (6) with $b=qB'(q)$. Note that Eq. (9) also implies that there is no constant FSC to $\langle N_b\rangle$.

It follows from finite-size scaling theory [15] that

$$C_{2b}=\langle N_b^2\rangle-\langle N_b\rangle^2=n_{2b}LL'+c_2L^{2/\nu}+\cdots. \tag{11}$$

The CFT result therefore suggests that

$$\langle N_c^2\rangle-\langle N_c\rangle^2=n_{2c}LL'+g^2c_2L^{2/\nu}+\cdots, \tag{12}$$

$$\langle N_cN_b\rangle-\langle N_b\rangle\langle N_c\rangle=n_{cb}LL'-gc_2L^{2/\nu}+\cdots. \tag{13}$$

It follows from Eqs. (5), (11), (12), and (13) that $a_2 = n_{2c} + g^2 n_{2b} + 2g n_{cb}$. Now we proceed to test the above predictions.

In [16], the internal energy of the Ising model on a large $L' \times L$ square lattice at the critical point, $U_I(T_c)/J_I$, is given by

$$-U_I(T_c)/J_I = \sqrt{2} + 2\Theta/L + d'/L^2 + \cdots, \tag{14}$$

where $\Theta = \theta_2\theta_3\theta_4/(\theta_2+\theta_3+\theta_4)$, J_I is the coupling constant of Ising spins and is related to J by $J = 2J_I$, θ_2, θ_3, and θ_4 are elliptic θ functions defined by Eq. (3.14) of [16] and d' was not determined in [16]. We have extended the expansion of $-U_I(T_c)/J_I$ up to order $1/L^3$ and find

$$-\frac{U_I}{J_I} = \sqrt{2} + \frac{2}{L}\Theta - \frac{2}{L^3}A_1\{p_1A_2 + p_2A_3 + p_3A_4\} + O\left(\frac{1}{L^4}\right), \tag{15}$$

where $A_1 = \theta_2\theta_3\theta_4$, $A_2 = 2\theta_2 + \theta_3 + \theta_4$, $A_3 = \theta_3 - \theta_4$, $A_4 = \theta_3 + \theta_4$,

$$p_1 = \frac{\pi^3 R}{2}\left(\sum_{l=1}^{\infty}\frac{1}{\sinh^4 \pi R l} + \frac{1}{9} + \frac{4(2-k^2)}{9\pi^2}K^2(k) - \frac{4}{3\pi^2}K(k)E(k)\right), \tag{16}$$

$$p_2 = \frac{\pi^3 R}{2}\left(\sum_{l=1}^{\infty}\frac{\cosh \pi R l}{\sinh^4 \pi R l} + \frac{1+k^2}{18\pi^2}K^2(k) - \frac{1}{72}\right), \tag{17}$$

and $p_3 = \pi^3 R/96$ with $K(k)$ and $E(k)$ the complete elliptic integrals of the first and second kind, respectively. The aspect ratio (R) and the modulus (k) of the elliptic functions are related to each other by $R = K(k')/K(k)$ with $k' = \sqrt{1-k^2}$.

Equation (15) shows that d' is zero, as predicted by Eq. (9). Since $U_I(T_c) = 2J_I + U$ and $U = -(\partial/\partial\beta)\ln Z_N/N = -(zJ/2p)\bar{p}$, $\bar{p} = \langle N_b\rangle/E$ and $n = \langle N_c\rangle/N$ are given by

$$\bar{p} = \frac{1}{2} + \frac{p_c\Theta}{2L} + \frac{p_c}{2L^3}A_1\{p_1A_2 + p_2A_3 + p_3A_4\} + O\left(\frac{1}{L^3}\right), \tag{18}$$

$$n = n_c - \frac{p_c}{2}\frac{\Theta}{L} + \frac{b}{L^2} + O\left(\frac{1}{L^3}\right), \tag{19}$$

where $\langle N_b\rangle$ and $\langle N_c\rangle$ satisfy Eq. (6). As another test of Eq. (9), we plot our $\bar{p}$ data for a square lattice three-state Potts model as a function of $L^{1/\nu-2} = L^{-0.8}$ in Fig. 2, which shows that the data fit a linear curve with slope $s = 0.1273 \pm 0.0005$. In Fig. 3 we plot $n - n_c$ data for the Ising model and three-state Potts model as a function of $1/L$ for $R = L'/L = 1$ and 2. The solid lines represent Eq. (19). The dotted line represents $n - n_c = -s/L^{0.8} + b/L^2$ with $b = 1.057\,79\ldots$ obtained via [14]. The agreement between the numerical data and our predictions is very good.

From [16] and the connection between the specific heat and the bond fluctuations, C_{2b}, of the QBCPM [9], we find that at the critical point p_c of the Ising model $c_{2b} = C_{2b}/LL' = c_2 \ln L + n_{2b} + O(1/L^2)$. Here $c_2 = 2p_c^2/\pi = 0.218\,453\ldots$, $n_{2b} = \frac{1}{4}p_c^2 B(0,R)/K_I^2 + 1/(\sqrt{2}+1)$, and $B(0,R)$ is defined by Eq. (4.21) of [16]; for $R = 1$, $n_{2b} = 0.475\,235\ldots$. Let $c_{2c} = (\langle N_c^2\rangle - \langle N_c\rangle^2)/LL'$ and $c_{bc} = (\langle N_c N_b\rangle - \langle N_b\rangle\langle N_c\rangle)/LL'$. For the Ising model (three-state Potts model), we fit c_{2b}, c_{2c}, and c_{bc} as linear functions of $\ln L (L^{1/\nu-2} = L^{0.4})$ to obtain n_{2b}, n_{2c}, and n_{bc} and slopes. $c_{2b} - n_{2b}$, $c_{2c} - n_{2c}$, and $c_{bc} - n_{bc}$ for the $L \times L$ Ising model as a function of $\ln L$ are shown in Fig. 4(a). The numerical values of c_2 and n_{2b} are 0.21(8) and 0.47(6), respectively, which are consistent with exact values. The slopes for c_{2c} and c_{bc} are 0.06(0) and $-0.11(5)$, respectively, which are consistent with Eqs. (12) and (13). $c_{2b} - n_{2b}$, $c_{2c} - n_{2c}$, and $c_{bc} - n_{bc}$ for three-state Potts model as a function of $L^{1/\nu-2} = L^{0.4}$ are shown in Fig. 4(b); the slopes of these curves are 0.64(3), 0.16(6), and $-0.32(7)$, respectively, which are also consistent with Eqs. (11)–(13).

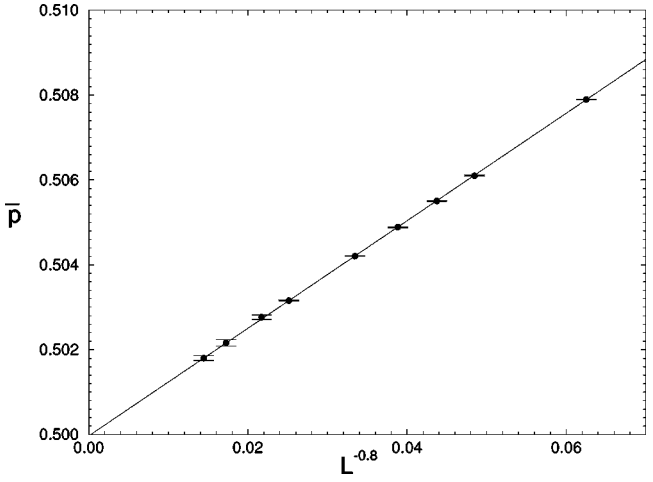

FIG. 2. Numerical $\bar{p}$ of square lattice three-state Potts model as a function of $L^{1/\nu-2}$ with $\nu = 5/6$ for three-state Potts model. The solid line represents $\bar{p} = 0.5 + s/L^{0.8}$ with $s = 0.127(3)$.

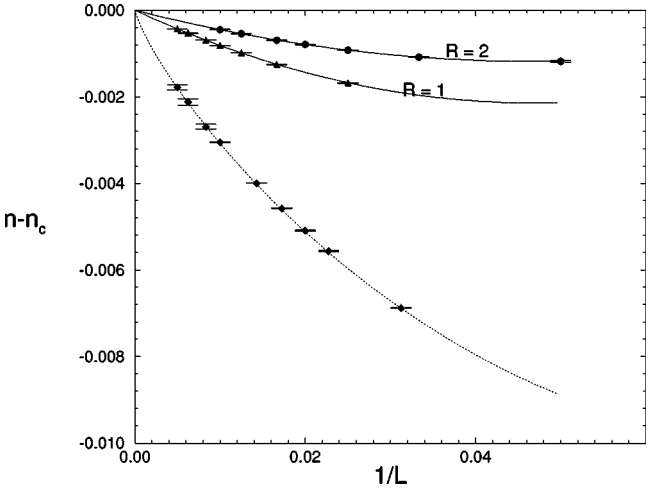

FIG. 3. Numerical $n - n_c$ of the $L' \times L$ square lattice Ising model and three-state Potts model as a function of $1/L$. The solid line represents Eq. (19) for the Ising model with $b(1) = 0.967\,734\ldots$ and $b(2) = 1.064\,63\ldots$. The dotted line represents the equation $n - n_c = -s/L^{0.8} + b/L^2$ for the three-state Potts model with $s = 0.127(3)$ and $b = 1.057\,79\ldots$.

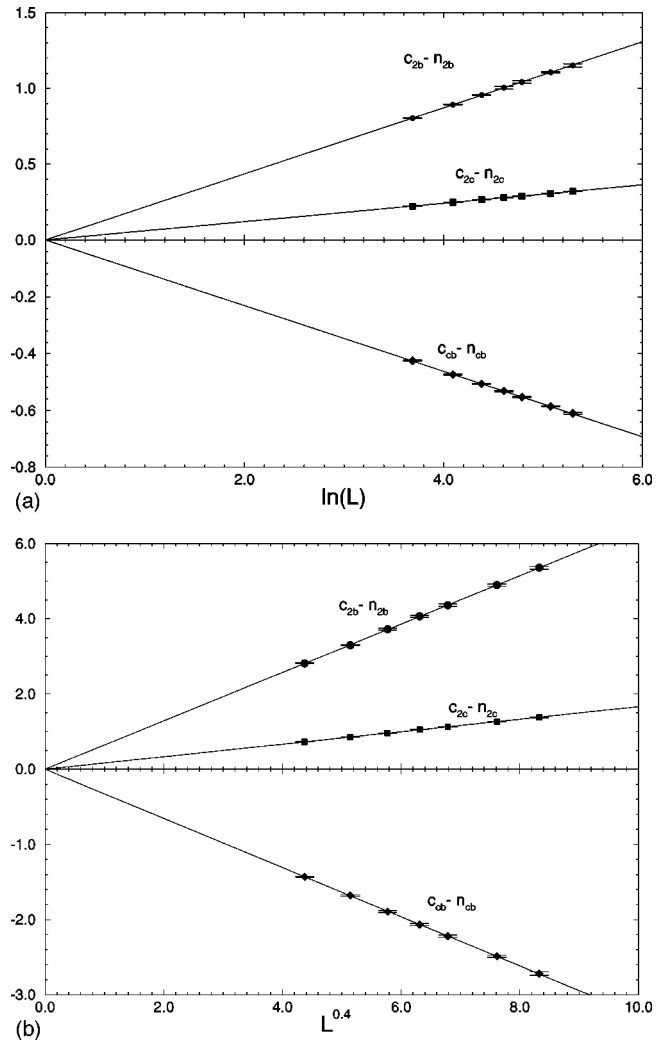

FIG. 4. (a) $c_{2b}-n_{2b}$, $c_{2c}-n_{2c}$, and $c_{bc}-n_{bc}$ for the Ising model as a function of $\ln L$, (b) $c_{2b}-n_{2b}$, $c_{2c}-n_{2c}$, and $c_{bc}-n_{bc}$ for the three-state Potts model as a function of $L^{2/\nu-2}=L^{0.4}$.

As $q\to 4$, the system approaches a multicritical point. From a RG point of view, its singular behavior may be understood in terms of a dilution field ψ and temperature field ϕ [17]. Since $\psi\sim\epsilon=(4-q)^{1/2}$, it follows from scaling theory that F_u will have an expansion in terms with integer powers of ϵ along the line of critical points. Thus b, which is proportional to the q derivative of F_u, and all higher cumulants b_n diverge as $q\to 4$. This agrees with the results of a direct calculation using [14], including the correct ϵ dependence. For the cylinder geometry, b is finite but b_n diverges for $n\geqslant 2$, which is attributable to the vanishing of the leading term in the expansion of F_u in this geometry.

For $q=4$, one cannot derive results for the FSC to $\langle N_c\rangle$ by differentiation. However, extending the scaling calculation in [18], we find that to leading order

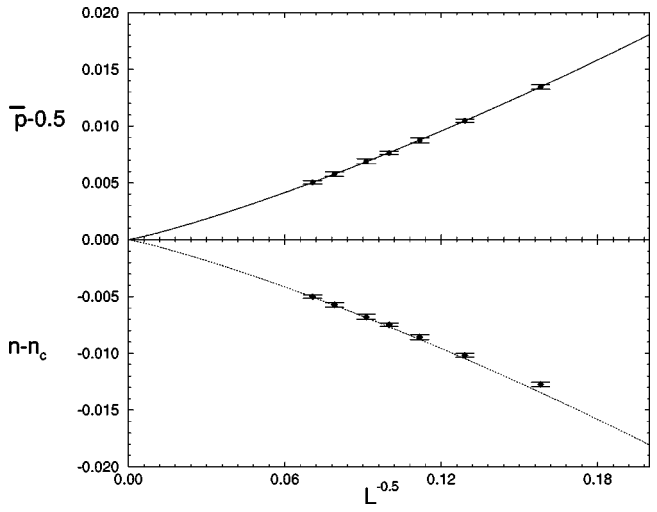

FIG. 5. $\bar{p}-0.5$ and $n-n_c$ for the four-state Potts model as a function of $x=L^{-1/2}$. The solid and dotted lines represents $w(x)$ and $-w(x)$, respectively.

$$\bar{p}=\langle N_b\rangle/E\approx 0.5+Ax(1-2a\ln x)^{-3/4}=0.5+w(x), \tag{20}$$

where $x=L^{1/\nu-2}$ with $\nu=2/3$ for the four-state Potts model [2], A and a are nonuniversal constants, and the square lattice bulk value $\bar{p}=0.5$ has been used. The FSC part of this result includes the effects of the constant term in the scaling relation for the free energy [18]. In Fig. 5, we plot data of $\bar{p}-0.5$ and $n-n_c$ for the four-state Potts model [13] as a function of $x=L^{-0.5}$. Fitting $\bar{p}-0.5$ to $w(x)$ of Eq. (20) gives $A=0.17\pm 0.01$ and $a=0.41\pm 0.05$. The solid and dotted lines in Fig. 5 represent $w(x)$ and $-w(x)$, respectively. Since $E=2LL'$ on the square lattice, Fig. 5 shows that $-w(x)$ also gives the leading FSC to $n-n_c$, which is similar to the cases $q=2$ and 3, i.e., we have numerical evidence for the relation $N_c\approx -gN_b$ when $q=4$.

Besides the Potts model, cluster representations are also useful for understanding critical properties of a model of hydrogen bonding in water, a dilute Potts model, the O(n) model, quantum spin models, and many others [9,19]. Our methods are useful for understanding finite-size corrections in these systems.

We are indebted to I. Affeck, A. Aharony, J. L. Cardy, M. E. Fisher, E. V. Ivashkevich, I. Peschel, P. Upton, F. Y. Wu, and R. M. Ziff for useful discussions. This work was supported in part by the National Science Council of the Republic of China (Taiwan) under Grant No. NSC 88-2112-M-001-011.

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