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

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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 \( < N_c > \) of the QBCPM has an energy-like 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, \( < N_b > \), has no constant term and explains the divergence of related quantities as \( q \rightarrow 4 \), the multicritical point. Similar analyses are applicable to a variety of other systems.

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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 [1], finite-size scaling functions [3], excess cluster numbers [1,4], etc. In a recent Letter, 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 $n = n_c + b/N + \ldots$, 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 non-trivial 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 $< N_c >$ is linearly related to the FSC for $< N_b >$, i.e. surprisingly, the number of clusters has an energy-like singularity. This is quite different from the case $q = 1$, which is equivalent to bond random percolation [10] studied by Ziff et al. [3,4]. Numerical simulation, scaling theory for the infinite system, and finite-size scaling arguments verify and illuminate this conclusion. The latter also implies that $< N_b >$ has no constant finite-size scaling term at criticality, which we verify explicitly for the Ising model on a square (sq) lattice. We also find that the FSC of $< N_c + gN_b >$ and its higher cumulants (where $g$ is defined below, and $g = 1/2$ for a sq 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 QBCPM and the QPM \[9,11\]. In the QPM, each site of the lattice \(G\) is occupied by a spin \(s_i\) with spin components \(-s, -s + 1, ..., s - 1, s\), where \(1 \leq i \leq N\), \(2s + 1 = q\), and \(q\) is an integer. The Hamiltonian of the QPM is given by

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

(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 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

\[
\pi(G', p, q) = p^{N_b(G')}(1 - p)^{E - N_b(G')} q^{N_c(G')},
\]

(2)

where \(p = 1 - \exp(-K) = 1\); the spontaneous magnetization \(M\) and the magnetic susceptibility \(\chi\) 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 \[8\]. The partition function of the QPM at zero magnetic field may be written as

\[
Z_N = \sum_{G'} (\exp(K) - 1)^{N_b(G')} q^{N_c(G')} = \exp(K E) \sum_{G'} \pi(G', p, q).
\]

(3)

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 bond, \(\bar{p}\), and the fluctuations of the number of occupied bonds, \(C_{2b}\), of the QBCPM, respectively \[8\].

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 $b = 0.884 \pm 0.002$, which are consistent with the result of Ziff et al. \[6\,7\]. However, results for $q = 2, 3, \text{and } 4$ are quite different, namely the curves for $q \geq 2$ have negative slopes, which suggests that the argument of Ziff et al. \[3\] 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 $q \geq 2$, consider the partition function $Z_c$ of the planar lattice QPM at the critical point $p_c = 1 - e^{-K_c}$:

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

Here $f(q) = e^{K_c} - 1$ and is known exactly for square, planar triangular, and honeycomb lattices \[3\]; for sq lattice, $f(q) = \sqrt{q}$. $Z_c$ is supposed to factor as $Z_c = Z_n Z_u$, 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 $N_c + g N_b$ are given by $C_n = [q(\partial/\partial q)]^n \ln Z_c$, where $g = g(q) = q f'(q)/f(q)$ and is $1/2$ for the sq lattice. Since $Z_u = Z_u(L'/L)$, FSC’s to $C_n$ are scale invariant. Thus, as in \[7\] for $q = 1$

$$C_n = a_n LL' + b_n (L'/L) + O(1/L),$$  \hfill (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

$$C_1 = <N_c + g N_b> = a_1 LL' + b(L'/L) + O(1/L).$$  \hfill (6)

For $q = 2$, $b(1) = 0.967734 \ldots$ and $b(2) = 1.06463 \ldots$; for $q = 3$, $b(1) = 1.05779 \ldots$ and $b(2) = 1.13321 \ldots$. Since $< N_b >$ 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 $< N_c >$ has an energy-like singularity with amplitude $-g$ times the amplitude of $< N_b >$. 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 $\alpha$ is the specific heat exponent. Differentiating $f_s$ with respect to $q$, we find $< N_c > \approx -A(q)p_c'(q)[p - p_c(q)]^{1-\alpha(q)}LL'$, showing that $< N_c >$ is energy-like 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

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

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

Here $\beta_c$, $\nu$, $B$, $C$, 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 $< N_c > = q(\partial/\partial q)lnZ_N$, $< N_b > = x(\partial/\partial x)lnZ_N$, we find for $\beta = \beta_c$ that

$$< N_c(G') > \approx n_c LL' - \frac{qf'(q)}{J(x_c + 1)}CL^{1/\nu} + qB'(q),$$

$$< N_b(G') > \approx n_b LL' + \frac{f(q)}{J(x_c + 1)}CL^{1/\nu}.$$ (8)

Note that exact results for $n_b$ are available and $n_b = 1$ for the sq lattice Potts model for any $q$ [3]. Therefore,

$$C_1 = < N_c + gN_b > = a_1 LL' + qB'(q),$$

(10)

where $a_1 = n_c + gn_b$, which agrees with Eq.(3) with $b = qB'(q)$. Note that Eq.(3) also implies that there is no constant FSC to $< N_b >$. 


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

\[ C_{2b} = \langle N_b^2 \rangle - \langle N_b \rangle^2 = n_{2b} L L' + c_2 L^{2/\nu} + \ldots. \]  

(11)

The CFT result therefore suggests that

\[ \langle N_c^2 \rangle - \langle N_c \rangle^2 = n_{2c} L L' + g^2 c_2 L^{2/\nu} + \ldots, \]  

(12)

\[ \langle N_c N_b \rangle - \langle N_b \rangle \langle N_c \rangle = n_{cb} L L' - g c_2 L^{2/\nu} + \ldots. \]  

(13)

It follows from Eqs. (5), (11), (12), and (13) that \( a_2 = n_{2c} + g^2 n_{2b} + 2 g n_{cb} \). 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

\[ -\frac{U_I}{J_I} = \sqrt{2} + \frac{2}{L} \Theta - \frac{2}{L^3} \Theta \Theta_1 + O \left( \frac{1}{L^4} \right), \]  

(14)

where

\[ \Theta = \frac{\theta_2 \theta_3 \theta_4}{\theta_2 + \theta_3 + \theta_4} \quad \text{and} \quad \Theta_1 = \frac{\pi^3 R \theta_2^9 + \theta_3^9 + \theta_4^9}{96 \theta_2 + \theta_3 + \theta_4} \]  

(15)

The aspect ratio \( (R) \) and the modulus \( (k) \) of the complete elliptic integrals of the first kind \( (K(k)) \) are related to each other by \( R = K(k')/K(k) \) with \( k' = \sqrt{1-k^2} \).

Equation (14) shows that \( d' \) is zero, as predicted by Eq.(5). Since \( U_I(T_c) = 2 J_I + U \) and \( U = -\frac{\partial}{\partial \beta} \ln Z_N/N = -\frac{\partial}{\partial \beta} \tilde{p} \), \( \tilde{p} = <N_b>/E \) and \( n = <N_c>/N \) are given by

\[ \tilde{p} = \frac{1}{2} + \frac{p_c \Theta}{2L} + \frac{p_c}{2L^3} \Theta \Theta_1 + O \left( \frac{1}{L^3} \right), \]  

(16)

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

(17)
where \( <N_b> \) and \( <N_c> \) satisfy Eq.(1). As another test of Eq.(3), we plot our \( \bar{p} \) data for square lattice three-state Potts model as a function of \( L^{1/v-2} = L^{-0.8} \) 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. (17). The dotted line represents \( n-n_c = -s/L + b/L^2 \) with \( b = 1.05779\ldots \) obtained via [14]. The agreement between 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 [3], we find that at the critical point \( p_c \) of the Ising model \( c_{2b} = C_{2b}/LL' = c_2 \ln L + n_{2b} + O \left( \frac{1}{L^2} \right) \). Here \( c_2 = 2p_c^2/\pi = 0.218453 \ldots \), \( n_{2b} = \frac{1}{4}p_c^2 B(0, R)/K^2_1 + 1/(\sqrt{2} + 1) \), and \( B(0, R) \) is defined by Eq.(4.21) of [16]; for \( R = 1 \), \( n_{2b} = 0.475235 \ldots \). Let \( c_{2c} = (<N_c^2> - <N_c>^2)/LL' \) and \( c_{bc} = (<N_cN_b> - <N_b><N_c>)/LL' \). For the Ising model (three-state Potts model), we fit \( c_{2b}, c_{2c}, \) and \( c_{bc} \) as linear functions of \( \ln L \) \( (L^{1/v-2} = L^{0.4}) \) 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 \( L^{1/v-2} = L^{0.4} \) 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).

As \( q \to 4 \), the system approaches a multicritical point. From an RG point of view, its singular behavior may be understood in terms of a dilution field \( \psi \) and temperature field \( \phi \) [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 \( \epsilon \) 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 \( \epsilon \) dependence. For the cylinder geometry, \( b \) is finite but \( b_n \) diverges for \( n \geq 2 \), 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 $< N_c >$ by differentiation. However, extending the scaling calculation in [18], we find that to leading order

$$
\bar{p} = < N_b > / E \approx 0.5 + A x (1 - 2a \ln x)^{-3/4} = 0.5 + w(x),
\tag{18}
$$

where $x = L^{1/\nu - 2}$ with $\nu = 2/3$ for four-state Potts model [2], $A$ and $a$ are non-universal constants and the sq 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 four-state Potts model [13] as a function of $x = L^{-0.5}$. Fitting $\bar{p} - 0.5$ to $w(x)$ of Eq.(18) 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 sq 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.

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FIGURES

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

FIG. 2. Numerical $\bar{p}$ of sq 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 $L' \times L$ sq lattice Ising model and three-state Potts model as a function of $1/L$. The solid line represents Eq. (17) for the Ising model with $b(1) = 0.967734 \ldots$ and $b(2) = 1.06463 \ldots$. The dotted line represent the equation $n - n_c = -s/L^{0.8} + b/L^2$ for the three-state Potts model with $s = 0.127(3)$ and $b = 1.05779 \ldots$

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 $L^{2/\nu - 2} = L^{0.4}$.

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.
Fig. 1. Hu et al.
Fig. 2 Hu et al.
Fig. 3 of Hu et al.
Fig. 4(b) Hu et al.
Fig. 5 Hu et al.