Site-bond-correlated percolation and a sublattice dilute Potts model at finite temperatures

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It is shown that the partition function of a sublattice dilute q-state Potts model (SDQPM) for even positive integer q at finite temperatures is the generating function of a site-bond-correlated percolation model (SBCPM) which favors subgraphs with larger numbers of disconnected finite clusters. The phase diagrams for the SBCPM are obtained from the corresponding phase diagrams for the SDQPM. A device is introduced to establish the connection between the SDQPM for $q \rightarrow 1$ and a site-bond (random) percolation model. The results of this work contain those of some previous papers as special cases.

I. INTRODUCTION

This is the sequel of a previous paper,¹ in which the connection between the thermal phase transition and the geometrical percolation transition was studied.² In establishing the connection between the Ising model (and other Ising-like spin models) and the correlated percolation model, we proposed¹ that one should consider the sites with a spin occupied and only the sites without a spin unoccupied. One should also regard the coupling between spins as a bond with a bond probability p, depending on the coupling strength J and the temperature T. In the illustrative example of the simple Ising model presented in that paper,¹ every lattice site is occupied by a spin- $\frac{1}{2}$ Ising spin, therefore the spin model corresponds to the bondcorrelated percolation model (BCPM). To demonstrate that our approach¹ can also be applied to the lattice spin model with vacant sites, in this we will apply our approach to a sublattice dilute q-state Potts model³ (SDQPM) which includes many Ising-like spin models $^{4-7}$ as special cases. In the SDQPM introduced in Ref. 3, some sites of one of the two sublattices are vacant. Using the general idea of Ref. 1, we will formally show that the partition function of the SDQPM at any temperature is the generating function of a site-bond-correlated percolation model (SBCPM) in which the vacant sites in the SBCPM correspond to the unoccupied sites in the SDQPM and the bond probability depends on the temperature and the coupling strength between occupied sites in the SDQPM. In the limit that every site is occupied, the SDQPM reduces to the decorated Potts model for the "case-1 lattice" in Ref. 3 or Potts model for the "case-2 lattice" in Ref. 3, and the SBCPM reduces to a purely bond-correlated percolation model. In the limit $T \rightarrow 0$, SBCPM reduces to the correlated percolation model defined in Sec. 3 of Ref. 3. From the connection mentioned

above, we can give the phase diagram $^{4-7}$ of the SDQPM a new geometrical interpretation. The connection also provides a geometrical picture for phase transitions in the studied spin model.

This paper is organized as follows: In Sec. II the partition function and certain physical quantities for the SDQPM defined in Sec. 2 of Ref. 3 are expressed in terms of summations over subgraphs of the whole lattice G. In such expansions, both sites and bonds in G are allowed to be vacant, while in Ref. 3 only sites are allowed to be vacant. In Sec. III a site-bond-correlated percolation model is defined whose connection with the SDQPM is established by the result of Sec. II. The phase diagrams for the site-bond-correlated percolation on some lattices are obtained from the corresponding phase diagrams of the SDQPM. In Sec. IV we explore the physical implications of the connection established in previous sections and write a formula which may be used to calculate the mean number of finite clusters per site of the SBCPM from the analytically continued partition function of the SDOPM. In Sec. V we introduce a device to establish the connection between the SDQPM for $q \rightarrow 1$ and a site-bond (random) percolation model (SBPM). Using this connection, we obtain the phase diagram for the SBPM from the phase diagram of the SDQPM for $q \rightarrow 1$. The obtained phase diagram for the SBPM on the semidilute honeycomb lattice is the same as that obtained by other methods.^{5,8} The results of this paper are summarized and discussed in Sec. VI.

II. GRAPH EXPANSION FOR A SUBLATTICE DILUTE POTTS MODEL

Here we briefly review the sublattice dilute Potts model introduced in Ref. 3 and define notations which are not always the same as those of Ref. 3. Let us divide the lat-

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tice of a crystal into two mutually penetrating sublattices, called the A (i.e., M in Ref. 3) and D sublattice, respectively; their lattice points will be labeled by indices i and α , respectively. Two possible relations between A and D sublattices will be considered below. In case 1 the vertices of an original lattice G_0 are taken as the A sublattice and the lattice points at the middle of the bonds of G_0 are taken as the D sublattice, i.e., we have a decorated lattice with vertices as the A sublattice and decorated points as the D sublattice. In case 2 all vertices of G_0 are divided into two equivalent sublattices: the A and D sublattices, i.e., we have a semidilute lattice. Examples of case-1 and case-2 lattices are shown in Figs. 1 and 7 of Ref. 4, respectively. Let N_a and N_d be the total number of sites on the A and D sublattices, respectively; then $N_d/N_a = c/2$ in the thermodynamic limit, where c equals z (z represents the coordination number for vertices of G_0) for decorated (i.e., case-1) lattices and 2 for semidilute (i.e., case-2) lattices.

Now we assign spin variables to lattice points. Every lattice point of the A and D sublattice is always occupied by a q-component spin s with spin components $j, j - 1, \ldots, -(j - 1), -j$, where 2j + 1 = q and q is a positive even integer. In addition to spin s, every lattice point of the D sublattice is also associated with a random variable t_{α} which can only be 0 or 1. When $t_{\alpha} = 0$ the spin s_{α} is eliminated. The Hamiltonian of the system is defined as

$$-H/kT = K \sum_{(i,\alpha)} t_{\alpha} \delta(s_{\alpha}, s_{i}) + \Delta \sum_{\alpha} t_{\alpha} + B_{1} \sum_{i} s_{i}$$
$$+ B_{2} \sum_{\alpha} t_{\alpha} s_{\alpha} . \qquad (1)$$

Here the first summation is a sum over all nearest neighbors. $\delta(s_{\alpha},s_i)=1$ or 0 when $s_{\alpha}=s_i$ or $s_{\alpha}\neq s_i$, respectively; K=J/kT is the normalized nearest-neighbor (NN) coupling constant. $\Delta=\mu/kT$ is the normalized chemical potential. B_1 and B_2 are normalized external magnetic fields applied to spins of the A and D sublattices, respectively, which will be set to 0 eventually. The partition function for the Hamiltonian of Eq. (1) can be written as

$$Z = \sum_{s_i = -j}^{j} \sum_{s_{\alpha} = -j}^{j} \sum_{t_{\alpha} = 0}^{1} \exp(-H/kT)$$

=
$$\sum_{s_i = -j}^{j} \sum_{s_{\alpha} = -j}^{j} \prod_{\alpha} (1 + e^{\Delta}) \prod_{(i,\alpha)} [1 + (e^{K} - 1)\delta(s_{\alpha}, s_i)]$$

$$\times \prod_{\alpha} e^{B_2 s_{\alpha}} \prod_{i} e^{B_1 s_i}, \quad (2)$$

where the second summation is over all sites with $t_{\alpha} = 1$, the first product is over all sites in the D sublattice, and where the primes on the second and third products indicate that the products extend over only those NN bonds or sites in which t_{α} assumes the value 1. Now we expand the first product in (2) and use the section graphs G' of G(representing the whole lattice) to represent the terms in the expansion. In each G', there are $v(G') \alpha$ sites which are occupied by the exponential factor (corresponding to $t_{\alpha}-1$) e^{Δ} in the expansion, where $0 \le v(G') \le v(G) = N_d$, with N_d defined above. For a given G', there corresponds a subgraph $G^* \subseteq G$ which is generated from G' by attaching bonds to every pair of the NN occupied sites in G'. We expand the second product in Eq. (2) and use the subgraphs G'' of G^* to represent the terms in the expansion. In each G'' there are e(G'') bonds which are occupied by the factor $(e^{K}-1)\delta(s_{\alpha},s_{i})$ in the expansion, where $0 \le e(G'') \le e(G^*) = lv(G^*)$, with l being 2z/c. If a particular site α of the D sublattice and the bond (i, α) are occupied, the spins s_i and s_a are said to be in the same cluster. In general, if two spins can be connected through a series of occupied sites (of the D sublattice) and bonds in the sense just mentioned, they are said to be in the same cluster. A given subgraph G'' usually contains a large number of independent clusters that include isolated sites of the D sublattice, whose NN bonds are all vacant. For a given subgraph G'', we can sum over all spin states at sites with $t_{\alpha} = 1$, and in such a summation only the terms where all spins in the same cluster have the same spin component have nonzero contributions. It should be noted that in nonzero terms, the spins in different clusters could have different spin components. Thus Eq. (2) can be written as

$$Z = \sum_{G' \subseteq G} e^{\Delta \nu(G')} \sum_{G'' \subseteq G^*} (e^K - 1)^{e(G'')} \prod_c \left[\exp(B_1 n_c + B_2 n_c') j + \exp(B_1 n_c + B_2 n_c') (j - 1) + \cdots + \exp(B_1 n_c + B_2 n_c') (-j) \right],$$
(3a)

where the product extends over all independent clusters of G'', and n_c and n'_c are numbers of spins which are in cluster c and belong to the A and D sublattices, respectively. Since $e(G^*) = lv(G')$, it is easy to show that Eq. (3a) can be rewritten as:

$$Z = (e^{\Delta + KI} + 1)^{v(G)} \sum_{G' \subseteq G} p_s^{v(G')} (1 - p_s)^{v(G) - v(G')} \sum_{G'' \subseteq G^*} p_b^{e(G'')} (1 - p_b)^{e(G^*) - e(G'')}$$

$$\times \prod_c \left[\exp(B_1 n_c + B_2 n_c') j + \dots + \exp(B_1 n_c + B_2 n_c') (-j) \right],$$
(3b)

where

$$p_{s} = \frac{\exp(\Delta + Kl)}{1 + \exp(\Delta + Kl)},$$

$$p_{b} = 1 - \exp(-K),$$
(4a)
(4b)

with *l* being 2 and *z* for decorated and semidilute lattices, respectively. From Eq. (3), it is easy to derive various thermodynamic quantities of interest. For example, the spontaneous magnetization $M(G,q,p_s,p_b,A)$, $M(G,q,p_s,p_b,D)$ of the spins in the *A* and *D* sublattice, respectively, and the internal energy $U(G,q,p_s,p_b)$ are given by the equations

$$M(G,q,p_{s},p_{b},A) = \lim_{B_{1},B_{2}\to 0^{+}} \lim_{N_{a},N_{d}\to\infty} \frac{1}{N_{a}} \frac{\partial}{\partial B_{1}} \ln Z = \lim_{N_{a}\to\infty} W^{-1} \sum_{G'\subseteq G} \sum_{G''\subseteq G^{*}} \Pi(G',G'',q,p_{s},p_{b})(N_{e}/N_{a})j , \qquad (5)$$

$$M(G,q,p_{s},p_{b},A) = \lim_{B_{1},B_{2}\to 0^{+}} \lim_{N_{d}\to\infty} \frac{1}{N_{d}} \frac{\partial}{\partial B_{2}} \ln Z = \lim_{N_{d}\to\infty} W^{-1} \sum_{G'\subseteq G} \sum_{G''\subseteq G^{*}} \Pi(G',G'',q,p_{s},p_{b})(N'_{e}/N_{d})j , \qquad (6)$$

and

$$U(G,q,p_s,p_b) = \lim_{B_1,B_2 \to 0} \lim_{N_a,N_d \to \infty} -\frac{1}{N_a + N_d} \frac{\partial}{\partial \beta} \ln Z = -\frac{c\mu}{c+2} \overline{p}_s - \frac{2Jz}{(c+2)p_b} \overline{p}_b , \qquad (7)$$

where

$$\Pi(G',G'',q,p_s,p_b) = p_s^{\nu(G')}(1-p_s)^{\nu(G)-\nu(G')} p_b^{e(G'')}(1-p_b)^{e(G^*)-e(G'')} q^{n_f(G'')},$$
(8)

$$W = \sum_{G' \subseteq G} \sum_{G'' \subseteq G^*} \Pi(G', G'', q, p_s, p_b) , \qquad (9)$$

$$\bar{p}_s = \lim_{N_d \to \infty} (WN_d)^{-1} \frac{\partial}{\partial \Delta} \ln Z = \lim_{N_d \to \infty} \sum_{G' \subseteq G} \sum_{G'' \subseteq G^*} W^{-1} \Pi(G', G'', q, p_s, p_b) v(G') / N_d , \qquad (10)$$

$$\overline{p}_b = \lim_{N_d \to \infty} (WN_d l)^{-1} p_b \frac{\mathrm{d}}{\mathrm{d}K} \ln Z = \lim_{N_d \to \infty} \sum_{G' \subseteq G} \sum_{G'' \subseteq G^*} W^{-1} \Pi(G', G'', q, p_s, p_b) e(G'') / (N_d l) .$$

$$\tag{11}$$

In Eq. (8), $n_f(G'')$ is the total number of finite clusters in G''. The extended cluster is defined to be the cluster which extends from one side of G to the opposite side of G and becomes an infinite cluster when $N_a, N_d \rightarrow \infty$. N_e of Eq. (5) and N'_e of Eq. (6) are the total numbers of spins which are in one of the extended clusters in G'' and belong to the A and D sublattice, respectively. It should be noted that usually $M(G,q,p_s,p_b,A) \neq M(G,q,p_s,p_b,D)$. The average spontaneous magnetization of spins in both M and D sublattices is given by

$$M(G,q,p_s,p_b) = \lim_{N_a,N_d \to \infty} \left[M(G,q,p_s,p_b,A)N_a + M(G,q,p_s,p_b,D)N_d \right] / (N_a + N_d) .$$
(12)

It is clear from Eqs. (10) and (11) that \bar{p}_s is the average number of spins at each site of the *D* sublattice and \bar{p}_b is the average number of bonds connecting the NN sites of *A* and *D* sublattices.

III. A SITE-BOND-CORRELATED PERCOLATION MODEL

A. Definition

Now we consider a site-bond-correlated percolation process on the lattice (graph G) mentioned above, which contains both the A and the D sublattice. For a given even positive integer q, the site-bond-correlated percolation is defined as follows.

Proposition 1 (P1): The sites of the A sublattice are always occupied.

Proposition 2 (P2): The sites of the *D* sublattice are occupied with a site probability p_s . This process generates section graphs $G' \subseteq G$. Attaching bonds to each pair of the NN occupied sites of G' constitutes $G^* \subseteq G$.

Proposition 3 (P3): Whenever a site of the *D* sublattice is occupied, the bonds which connect this site with its *l* NN sites of the *A* sublattice are attached with a bond probability p_b . This process generates subgraphs $G'' \subseteq G^*$, where some bonds of G'' are vacant. The occupied sites connected through a series of occupied bonds and sites are said to be in the same cluster. Proposition 4 (P4): The overall probability of a subgraph $G'' \subseteq G^* \subseteq G$ is enhanced by a factor q for each finite cluster in G''.

For given G, q, p_s , and p_b , one might try to calculate the following quantities: (i) the probability $P(G,q,p_s,p_b,A)$ that a site of the A sublattice belongs to an infinite cluster, (ii) the probability $P(G,q,p_s,p_b,D)$ that a site of the D sublattice belongs to an infinite cluster, (iii) the probability $P(G,q,p_s,p_b)$ that an arbitrary site (including both sites of the A and D sublattices) belongs to an infinite cluster. It is obvious that expressions for $P(G,q,p_s,p_b,A)$, $P(G,q,p_s,p_b,D)$, and $P(G,q,p_s,p_b)$ are exactly the same as those for $M(G,q,p_s,p_b,A)/j$, $M(G,q,p_s,p_b,D)/j$, and $M(G,q,p_s,p_b)/j$. Thus they can be calculated from the corresponding quantities of the SDQPM.

From Eqs. (10) and (11), it is clear that \bar{p}_s is also the average number of occupied sites at each site of the *D* sublattice, and \bar{p}_b is the average number of attached bonds at each NN bond connecting sites of the *A* and *D* sublattices for the site-bond-correlated percolation model (SBCPM). If there is no enhanced factor of (P4), $\bar{p}_s = p_s$ and $\bar{p}_b = p_b$. The enhanced factor of (P4) favors subgraphs with larger numbers of finite clusters, hence usually $\bar{p}_s < p_s$ and $\bar{p}_b < p_b$ for $0 < p_s, p_b < 1$.

In (P3) only the bonds of G^* are attached with a bond probability p_b . Instead of using (P2) and (P3) above, if all sites of G are occupied with a site probability p_s and all bonds of G are attached with a bond probability p_b , so that the subgraphs G" are generated, then it is possible to have "unsaturated" attached bonds in G", whose end points are not completely occupied. However, such unsaturated bonds are irrelevant for the calculation of a physical quantity, e.g., the spontaneous magnetization, which does not depend on the unsaturated bonds.⁹

B. Phase diagrams

For the Hamiltonian of Eq. (1) with $B_2=0$ on the decorated (i.e., case-1) lattices, we can carry out the configuration summation of the decorated spins s_{α} and random variables t_{α} , $\alpha=1,\ldots,N_d$, to obtain an effective Hamiltonian

$$H_{\rm eff}/kT = K^* \sum_{\langle ij \rangle} \delta(s_i, s_j) + B_1 \sum_i s_i + K_0^* \sum_i \frac{z}{2} , \qquad (13)$$

on the original undecorated lattice G_0 . Here the first summation is a sum over all NN bonds of G_0 , and K^* and K_0^* are given by the equations⁶

$$\exp(K^*) = \frac{1 + e^{\Delta}(e^{2K} + q - 1)}{1 + e^{\Delta}(2e^K + q - 2)}, \qquad (14)$$

$$\exp(K_0^*) = 1 + e^{\Delta}(2e^K + q - 2) .$$
(15)

Equation (14) gives the phase diagram of the orderdisorder transitions for the SDQPM when K^* assumes the value of the critical coupling constant K_c^* for the system of Eq. (13). From Eqs. (4) and (14), we can rewrite such phase diagram in terms of p_s and p_b and have the phase diagram for the SBCPM:

$$(u_c+1)p_s[1-2(1-p_b)-(q-2)(1-p_b)^2 + (u_c+1)^{-1}(q-1)(1-p_b)^2] = u_c , \qquad (16)$$

where

$$u_c = \exp(K_c^*) - 1$$
. (17)

In the limit $T \rightarrow 0$, we have $p_b = 1$ and Eq. (16) reduces to

$$p_s = u_c / (u_c + 1)$$
 (18)

In the limit $\mu/J \rightarrow \infty$ we have $p_s = 1$ (i.e., no vacancy) and Eq. (16) reduces to

$$(u_{c}+1)[1-2(1-p_{b})-(q-2)(1-p_{b})^{2} + (u_{c}+1)^{-1}(q-1)(1-p_{b})^{2}] = u_{c} .$$
(19)

For the square (sq), plane triangular (pt), and honeycomb (hc) lattices, u_c is known rigorously.¹⁰ u_c for the sq lattice is given by

$$u_c(sq) = (q)^{1/2}$$
 (20)

 $u_c(\text{pt})$ and $u_c(\text{hc})$ can be obtained from the solution of the cubic equations

$$u_c^3 + 3u_c^2 - q = 0 \tag{21}$$

and

$$u_c^3 - 3qu_c - q^2 = 0 , \qquad (22)$$

respectively. With such exact values in Eq. (18) for q = 2, we obtain the critical point $p_{s,c} = 0.585786...$, 0.422 649..., and 0.732 050... for the decorated sq, pt, and hc lattices, respectively, which are consistent with results of Table I in Ref. 3.

The exact phase diagram for the SDQPM on the semidilute hc lattice has been calculated by Kondor and Temesvari⁵ and is given by

$$q^{2}e^{-\Delta}(e^{K}-1)^{-3}+3q^{2}(e^{K}-1)^{-2}+q^{3}(e^{K}-1)^{-3}=q.$$
 (23)

Using Eq. (4), we can transform Eq. (23) into the phase diagram for the SBCPM:

$$p_{s}[1-3p_{b}(1-p_{b})^{2}-q(1-p_{b})^{3}+q^{-1}p_{b}^{3}]=1.$$
 (24)

In the zero-temperature (i.e., $T \rightarrow 0$, $p_b \rightarrow 1$) or no-vacancy (i.e., $u/J \rightarrow \infty$, $p_s \rightarrow 1$) limits, Eq. (24) reduces to

$$p_s = q/(q+1) \tag{25}$$

or

$$1 - 3p_b(1 - p_b)^2 - q(1 - p_b)^3 + q^{-1}p_b^3 = 1 , \qquad (26)$$

respectively. For q=2, Eq. (25) gives the critical point $p_{s,c}=0.6666\ldots$, which is consistent with the value listed in Table I of Ref. 3. Equation (24) can be extended to the anisotropic case. If J_a (a=1,2,3) are the two-body couplings in the three directions on the hc lattice and $K_a=J_a/kT$, the critical condition is⁵

$$W + U_1 U_2 + U_2 U_3 + U_3 U_1 + U_1 U_2 U_3 = q$$
, (27)

where

$$U_{a} = q / [\exp(K_{a}) - 1] ,$$

$$W = \frac{q^{2} \exp(-\Delta)}{[\exp(K_{1}) - 1] [\exp(K_{2}) - 1] [\exp(K_{3}) - 1]}$$

Applying a procedure similar to that used to derive Eq. (3b), we may show that the partition function of the anisotropic SDQPM on the hc lattice may be written as the generating function of an anisotropic SBCPM on the hc lattice with bond probabilities p_{b1}, p_{b2}, p_{b3} , along three directions and the site probability p_s given by the equations

$$p_{b1} = 1 - \exp(-K_1)$$
, $p_{b2} = 1 - \exp(-K_2)$,
 $p_{b3} = 1 - \exp(-K_3)$, (28a)

$$p_{s} = \frac{\exp(\Delta + K_{1} + K_{2} + K_{3})}{1 + \exp(\Delta + K_{1} + K_{2} + K_{3})} .$$
(28b)

With Eq. (28), we can transform Eq. (27) into the phase diagram for the anisotropic SBCPM on the hc lattice:

$$p_{s}[(1-q)(1-p_{b1}-p_{b2}-p_{b3})+(2-q)(p_{b1}p_{b2}+p_{b2}p_{b3}+p_{b3}p_{b1})-(3-q-1/q)p_{b1}p_{b2}p_{b3}]=1.$$
(29)

The approximate phase diagrams for the SDQPM on the semidilute sq and simple cubic (sc) lattices for q = 2 have been

calculated by Hu and Kleban,⁷ using a renormalization group method.¹¹ With Eq. (4), we may transform such phase diagrams for the SBCPM on the semi-dilute sq and sc lattices.

IV. RELATIONS BETWEEN PERCOLATION AND THERMAL PHASE TRANSITIONS

One of the purposes of investigating the connection between correlated percolation models and spin models is to understand whether or not the phase transitions in spin models are related to percolation transitions of certain percolation processes. We have pointed out that the percolation probability of the SBCPM defined in Sec. III is proportional to the spontaneous magnetization of the SDQPM defined in Sec. II. Thus they have the same critical temperature T_c and exponent β . Following the procedure used in Ref. 1, we may use Eq. (3) to show that the magnetic susceptibility and spin-spin correlation function of the SDQPM are related to the mean cluster size and pair-connectedness function of the SBCPM. In particular, they have the same critical point and exponents γ (perhaps also γ' ; see Ref. 1 for a discussion), ν , ν' , and η .

In the following, we will use $[Q(G'')]_{av}$ to denote the mean value of a subgraph-dependent quantity Q(G'') averaged over all subgraphs $G'' \subseteq G^* \subseteq G$. Namely,

$$[Q(G'')]_{av} = W^{-1} \sum_{G' \subseteq G} \sum_{G'' \subseteq G^*} \Pi(G', G'', q, p_s, p_b) Q(G'') , \qquad (30)$$

where $\Pi(G', G'', q, p_s, p_b)$ and W are given by Eqs. (8) and (9), respectively. We will also use $\langle Q(G'') \rangle_0$ to denote the value $[Q(G'')]_{av}$ per site of the D sublattice in the thermodynamic limit, i.e.,

$$\langle Q(G'') \rangle_{0} = \lim_{N_{d} \to \infty} \left[Q(G'') \right]_{av} / N_{d} = \lim_{N_{d} \to \infty} W^{-1} \sum_{G' \subseteq G} \sum_{G'' \subseteq G^{*}} \Pi(G', G'', q, p_{s}, p_{b}) Q(G'') / N_{d} .$$
(31)

Using Eq. (7), we may show that the specific heat per spin of the SDQPM is given by

$$C(G,q,p_{s},p_{b}) = \frac{\partial}{\partial T} U(G,q,p_{s},p_{b}) = -\frac{2zkK^{2}e^{-K}}{(c+2)p_{b}^{2}} \overline{p}_{b} + \frac{ck}{c+2} \left[\Delta^{2} \langle [\delta v(G^{\prime\prime})]^{2} \rangle_{0} + \frac{2K\Delta}{p_{b}} \langle \delta v(G^{\prime\prime})\delta e(G^{\prime\prime}) \rangle_{0} + \frac{K^{2}}{p_{b}^{2}} \langle [\delta e(G^{\prime\prime})]^{2} \rangle_{0} \right],$$
(32)

where

$$v(G'') = v(G'') - [v(G'')]_{av}, e(G'') = e(G'') - [e(G'')]_{av}$$

Thus the specific heat is related to the fluctuations and cross fluctuations of v(G'') and e(G''). In particular, the former and the latter have the same critical temperature T_c and exponents α and α' .

The normalized (by kT) free energy per spin of the SDQPM for $B_1 = B_2 = 0$ in the thermodynamic limit may be calculated from Eq. (3). If we take the thermodynamic limit first and then set $B_1 = B_2 = 0$, we have

$$f(G,q,p_{s},p_{b}) = \lim_{B_{1},B_{2}\to 0} \lim_{N_{a},N_{d}\to\infty} \ln(Z)/(N_{a}+N_{d})$$

$$= \frac{c}{c+2} \ln[1+\exp(\Delta+Kl)] + \lim_{N_{a}N_{d}\to\infty} \ln\left(\sum_{G'\subseteq G} \sum_{G''\subseteq G^{*}} \Pi(G',G'',q,p_{s},p_{b})\right) / (N_{a}+N_{d}).$$
(33)

Now suppose we may analytically continue Eq. (33) from positive even integer q to any positive real q; the mean number of finite clusters per site of the SBCPM may be calculated formally from the equation

$$N_c(G,q,p_b) = q \frac{\partial}{\partial q} f(G,q,p_s,p_b) .$$
(34)

V. EXTENSION TO THE CASE $q \rightarrow 1$

Up to now, we have considered the SDQPM for q being a positive even integer, because in this case, we may write the partition function of the SDQPM in an external magnetic field in the form of Eq. (3). When we use Eq. (3) to calculate the spontaneous magnetization, only percolating clusters have nonzero contributions. Thus we may relate the spontaneous magnetization of the SDQPM to the percolation probability of the SBCPM defined in Sec. III.

Now we will introduce a device by which we may relate the SDQPM for $q \rightarrow 1$ to a SBPM. We still consider a lattice G consisting of two mutually penetrating sublattices A and D whose lattice sites are labeled by the indexes *i* and α , respectively. Each site of G is assigned a q-component spin s with spin components s = 1, 2, ..., q and each site of the D sublattice is also associated with a random variable t_{α} , which may only be 0 or 1. The Hamiltonian of the system is defined as

$$-H^*/kT = K \sum_{(i,\alpha)} t_{\alpha} \delta(s_{\alpha}, s_i) + \Delta \sum_{\alpha} t_{\alpha} + B_1 \sum_{i} \delta(s_i, 1) + B_2 \sum_{\alpha} \delta(s_{\alpha}, 1) .$$
(35)

The notations in Eq. (35) are the same as those in Eq. (1). The difference between Eqs. (1) and (35) should be noted. In Eq. (35), B_1 and B_2 couple only with the first component of s_i and s_{α} , respectively. The first and last terms of Eq. (35) indicate that the sites of the *D* sublattice with t=0 still have Potts spins which can couple with the external magnetic field B_2 , and the effect of taking $t_{\alpha}=0$ is just to decouple the Potts coupling of s_{α} with its nearest neighbors rather than to eliminate s_{α} completely. Using a procedure similar to that used to derive Eq. (3a), we may write the partition function for the Hamiltonian of Eq. (35) as follows:

$$Z^* = \sum_{G' \subseteq G} e^{\Delta v(G')} \sum_{G'' \subseteq G^*} (e^K - 1)^{e(G'')} \prod_{c^*} \left[\exp(B_1 n_{c^*} + B_2 n'_{c^*}) + q - 1 \right].$$
(36)

The meanings of G', G'', v(G'), and e(G'') are the same as those of Eq. (3). The sites connected through a series of attached bonds, and occupied sites of G' are said to be in the same cluster. The product extends over all clusters in G''considered in Eq. (3) and also the sites of the D sublattice with $t_{\alpha}=0$. n_{c^*} and n'_{c^*} are numbers of spins which are in cluster c^* and belong to the A and D sublattice, respectively. It is obvious that

$$\sum_{c^*} n_{c^*} = N_a \tag{37a}$$

and

$$\sum_{*} n'_{c*} = N_d . (37b)$$

Equation (37a) is also true for the clusters of Eq. (3a), but Eq. (37b) is not true for the clusters of Eq. (3a). Since $e(G^*) = lv(G')$, we may rewrite Eq. (36) as

$$Z^{*} = (e^{\Delta + Kl} + 1)^{\nu(G)} \sum_{G' \subseteq G} p_{s}^{\nu(G')} (1 - p_{s})^{\nu(G) - \nu(G')} \sum_{G'' \subseteq G^{*}} p_{b}^{e(G'')} (1 - p_{b})^{e(G^{*}) - e(G'')} \prod_{c^{*}} [\exp(B_{1}n_{c^{*}} + B_{2}n_{c^{*}}) + q - 1)].$$
(38)

where p_s and p_b are still given by Eqs. (4a) and (4b).

Following Wu's paper¹² in which the undilute q-state Potts model for $q \rightarrow 1$ was shown to correspond with the random bond percolation model, we write the free energy per site of the SDQPM as

$$f(G,q,K,\Delta,B_1,B_2) = \lim_{N_a,N_d \to \infty} \ln Z^* / (N_a + N_d)$$
(39)

and further define

$$h(G,K,\Delta,B_1,B_2) = \left[\frac{\partial}{\partial q}f(G,q,K,\Delta,B_1,B_2)\right]_{q=1}.$$
(40)

Interchanging the order of derivative and the thermodynamic limit and using the relations of Eqs. (37a) and (37b), we may easily show that

$$h(G,K,\Delta,B_1,B_2) = \lim_{N_a,N_d\to\infty} W^{-1} \sum_{G'\subseteq G} \sum_{G''\subseteq G^*} \Pi(G',G'',1,p_s,p_b) \sum_{c^*} [\exp(-B_1n_{c^*} - B_2n'_{c^*})/(N_a + N_d)].$$
(41)

where $\Pi(G', G'', 1, p_s, p_b)$ and W are just those of Eqs. (8) and (9) evaluated at q = 1, the summation is restricted to clusters of finite size (indicated by the prime sign) for any $B_1 > 0$ or $B_2 > 0$. It is clear that the mean number of finite clusters plus the number of vacant sites of the D sublattice per site is given by

$$N_{c}(G, p_{s}, p_{b}) = h(G, K, \Delta, B_{1} \to 0^{+}, B_{2} \to 0^{+}) .$$
(42)

The spontaneous magnetization $M(G, p_s, p_b, A)$ and $M(G, p_s, p_b, D)$ of the spins in the A and D sublattice, respectively, are given by

$$M(G, p_s, p_b, A) = 1 + \frac{2}{c+2} \left[\frac{\partial}{\partial B_1} h(G, K, \Delta, B_1, B_2 \to 0) \right]_{B_1 = 0^+}$$
$$= 1 - \lim_{N_a \to \infty} W^{-1} \sum_{G' \subseteq G} \sum_{G'' \subseteq G^*} \Pi(G', G'', 1, p_s, p_b) \left[\sum_{c^*} n_{c^*} \right] / N_a , \qquad (43)$$

and

$$M(G,p_s,p_b,D) = 1 + \frac{c}{c+2} \left[\frac{\partial}{\partial B_2} h(G,K,\Delta,B_1 \to 0^+,B_2) \right]_{B_2 = 0^+}$$
$$= 1 - \lim_{N_d \to \infty} W^{-1} \sum_{G' \subseteq G} \sum_{G'' \subseteq G^*} \Pi(G',G'',1,p_s,p_b) \left[\sum_{c^*} n'_{c^*} \right] / N_d .$$
(44)

It is obvious that $M(G,p_s,p_b,A)$ and $M(G,p_s,p_b,D)$ are just the percolation probability, that an arbitrary site of the A and D sublattice, respectively, belongs to an infinite (percolating) cluster of the SBPM defined by (P1)-(P3), but without (P4), of Sec. III. Following the procedure of Sec. IV, we may also relate the specific heat of the SDQPM for $q \rightarrow 1$ with the site and bond fluctuations and cross fluctuations of the SBPM just mentioned.

We may analytically continue the phase diagrams of the SBCPM [e.g., those of Eqs. (16), (24), and (29)] to obtain the phase diagrams of the SBPM. In particular, in the limit $q \rightarrow 1$, Eqs. (24) and (29) reduce to

$$p_s(3p_b^2 - p_b^3) = 1$$
, (45)

and

$$p_{s}(p_{b1}p_{b2}+p_{b2}p_{b3}+p_{b3}p_{b1}-p_{b1}p_{b2}p_{b3})=1, \quad (46)$$

respectively, which have been derived before^{8,5} using different methods.

VI. SUMMARY AND DISCUSSION

In Sec. II we have expressed the partition function and some physical quantities of the sublattice dilute q-state Potts model (SDQPM) (for a positive even integer q) on a lattice G, which is divided into A and D sublattices, in terms of subgraph expansions. Such expansions allow us to draw the connection between the SDQPM and a sitebond-correlated percolation model (SBCPM) defined in Sec. III A. We then use this connection to obtain phase diagrams for the SBCPM from phase diagrams for the SDQPM in Sec. III B and to relate the mean number of finite clusters per site of the SBCPM with the derivative of the free energy per site of the SDQPM with respect to qin Sec. IV. In Sec. V we introduce a device so that results of previous sections may be extended to the case $q \rightarrow 1$. In particular, from such extension, we have rederived the phase diagram of the site-bond (random) percolation model defined on the semidilute hc lattice, which was obtained by Kondor and Temesvari^{8,5} before, using different methods.

The results of Secs. II and III become those of Ref. 3 in the limit $T \rightarrow 0$, in which p_b of Eq. (4b) becomes 1 and the SBCPM defined in Sec. III A becomes the site-correlated

percolation model defined in Sec. 3 of Ref. 3. In the limit of no vacancy [i.e., Δ and K of Eq. (1) satisfy $\Delta/K \rightarrow \infty$], the SDQPM on the semidilute lattice become the undilute Potts model which contains the simple Ising model studied in Ref. 1 for the special case q = 2. Thus the results of Secs. II and III also contain results of Ref. 1.

The $\Pi(G', G'', q, p_s, p_b)$ of Eq. (33) is given by Eq. (8) and contains a *q*-dependent factor:

$$q^{n_f(G'')}$$
, (47)

where $n_f(G'')$ is the total number of finite clusters in G''. If we set $B_1 = B_2 = 0$ first and then take the thermodynamic limit, the q-dependent factor in Eq. (33) must be replaced by

$$q^{n_{f}(G'')}q^{n_{p}(G'')} = q^{n_{t}(G'')}, \qquad (48)$$

where $n_p(G'')$ is the total number of percolating clusters in G'' and $n_t(G'')=n_f(G'')+n_p(G'')$ is the total number of clusters in G''. The contribution to the sum over subgraphs, e.g., in Eq. (6), is expected to peak sharply on certain rather similar subgraphs G^* . The difference in the contributions of Eqs. (47) and (48) to the probability weight $\Pi(G', G'', q, p_s, p_b)$ is not very significant, because $n_p(G'') \ll n_f(G'')$ for T > 0 and previous studies indicate that $n_p(G^*) \le 1$ at least for lower space dimensions,¹³ e.g., d = 1-3.

The graph expansion of the SDQPM and its connection with the correlated percolation may be extended easily to many dilute and undilute spin models of half-integer spins, including the fully dilute *q*-state Potts model (FDQPM), the Baxter model, etc. Actually Wu has obtained the graph expansions for the partition function of the simple Potts model¹² and the FDQPM (Ref. 9) before. But he considered the connection between these models and percolation models only for the case $q \rightarrow 1$.

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- ⁴I. Syozi and S. Miyazima, Prog. Theor. Phys. <u>36</u>, 1083 (1966).
- ⁵I. Kondor and T. Temesvari, J. Phys. C <u>14</u>, L97 (1981).
- ⁶F. Y. Wu, J. Stat. Phys. <u>23</u>, 773 (1980).

¹C.-K. Hu, this issue, preceding paper Phys. Rev. B <u>29</u>, 5103 (1984).

²See Sec. I of Ref. 1 for a brief review of this field and related references.

³C.-K. Hu, Physica <u>116A</u>, 265 (1982). The author found that in this paper Q of Eq. (5) should be j rather than q/4 and q/2 of

Eq. (7) should be replaced by 1 with a corresponding change in the definition of the correlated percolation problem in Sec. III.

- ⁷C.-K. Hu and P. Kleban, Phys. Rev. B <u>25</u>, 6760 (1982).
- ⁸I. Kondor, J. Phys. C <u>13</u>, L531 (1980).
- ⁹See p. L42 of F. Y. Wu, J. Phys. A <u>14</u>, L39 (1981).
 ¹⁰F. Y. Wu, Rev. Mod. Phys. <u>54</u>, 235 (1982).
- ¹¹C.-K. Hu and P. Kleban, J. Comp. Phys. <u>43</u>, 289 (1981).
- ¹²F. Y. Wu, J. Stat. Phys. <u>18</u>, 115 (1978).

¹³C. M. Newman and L. S. Schulman, J. Phys. A <u>14</u>, 1735 (1981) and references therein; H. Nakanishi and H. E. Stanley, ibid. 14, 693 (1981) (see footnote on page 695; although the percolation model here is different from ours, similar results might be expected in our model).