

## Percolation Theory of Phase Transitions in Spin Models\*

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The phase transition in the spin model and the percolation transition in the lattice percolation model have many characteristics in common which have motivated researchers to explore whether the former is a percolation transition of a correlated percolation model. Previous attempts to draw such a connection have been either unsuccessful or unsatisfactory. This paper briefly reviews a new approach which not only solves the problem but also provides a new avenue to understand the behavior of phase transitions in spin models.

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## I. INTRODUCTION

**T**HIS morning Professor Prigogine<sup>1</sup>, who won the Nobel Prize in Chemistry in 1977, delivered lectures on nonequilibrium statistical mechanics. This afternoon, Professor Eu<sup>2</sup> and Professor Mou<sup>3</sup> from chemistry departments gave lectures on transport process which is an important problem of statistical physics. Now I will present a talk on percolation which is also a statistical mechanical problem attracting both chemistry and physics people. Although Professor Flory of the chemistry department of Cornell University did not use the technical term "percolation", in 1941 he first used the concept of percolation to describe a nonequilibrium phase transition process, namely the sol-gel transition of polymers<sup>4</sup>. In 1957, Professor Hammersley and Professor Broadbent<sup>5</sup> advocated the concept of percolation and introduced the technical term "percolation". Now percolation has been growing into an important branch of statistical physics. Many physical processes seem to relate to percolation problems as can be seen from the table of contents of a recent book<sup>6</sup>: "Percolation Structures and Processes."

Today I will address on a particular problem of percolation. Namely, the connection between the percolation transition and the phase transition in spin models. The essential question here is: "whether the phase transition in a spin model is a kind of percolation transition?". This question has puzzled

many scientists since 1974. Now I think I have solved the problem<sup>7-9</sup>, my answer to the question is: "Yes! the phase transition in a spin model is a kind of percolation transition." Furthermore, from this connection, we are able to physically understand many properties of spin models<sup>10-12</sup>.

## II. BASIC PERCOLATION CONCEPTS

To begin with, let me first review basic ideas of percolation processes on a  $d$ -dimensional lattice  $G$  with  $N$  sites and  $E$  bonds, such as the square lattice of Fig. 1. In the bond random percolation for a given bond probability  $P_b$ , each bond of  $G$  is attached with the probability  $P_b$ . The probability weight for a given subgraph  $G' \subseteq G$  of  $b(G')$  attached bonds and  $E-b(G')$  vacant (i.e. unattached) bonds to appear is simply given by:

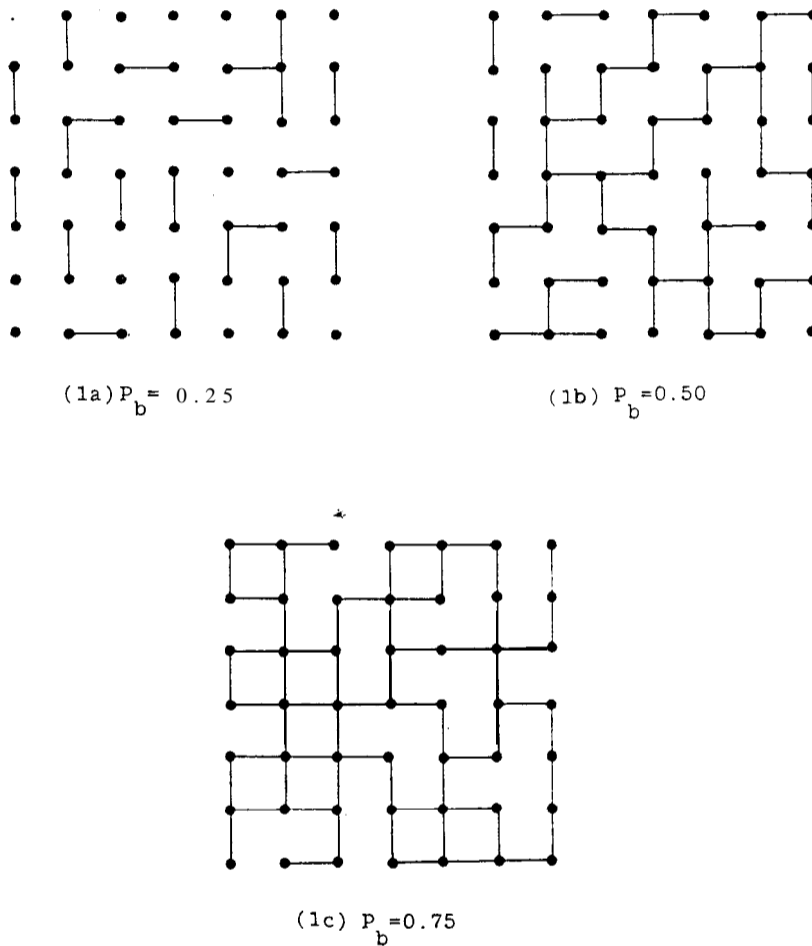


Fig. 1 Bond percolation on a square lattice. The bond probabilities  $P_b$  for Fig. 1a, 1b, and 1c are 0.25, 0.50, and 0.75, respectively. The attached bonds are represented by solid (—) lines. The sites connected by a sequence of solid lines are said to be in the same cluster.

$$\pi(G', P_b) = P_b^{b(G')} (1 - P_b)^{E-b(G')} \quad (2.1)$$

By definition, the sites connected by attached bonds are said to be in the same cluster. The isolated sites, i.e. sites without any attached bonds, are one-site cluster. Based on Eq. (2.1), we may use the Monte Carlo simulation method to generate a Markovian chain of subgraphs. For a large  $N$ , certain rather similar subgraphs  $G^*$ , called dominant subgraphs, dominate in the Markovian chain when the system is in equilibrium. For very small  $P_b$  (Fig. 1a), the dominant subgraphs have only small and isolated clusters, when  $P_b$  is increased, the dominant subgraphs contain larger and larger subgraphs. When  $P_b$  reaches a critical value  $P_{b,c}$  (Fig. 1b), the dominant subgraphs begin to contain the percolating cluster which extends from one side of the lattice to another. When  $P_b$  is increased from  $P_{b,c}$ , percolating clusters contain a finite fraction of total lattice site (Fig. 1c). The transition from subgraphs without percolating clusters to subgraphs with percolating clusters is called the percolation transition.

In the site random percolation on  $G$ , each site of  $G$  is occupied with the probability  $P_s$ . The probability weight for a given subgraph  $G'$  of  $v(G')$  occupied sites and  $N-v(G')$  vacant sites is given by:

$$\pi(G', P_s) = P_s^{v(G')} (1 - P_s)^{N-v(G')} \quad (2.2)$$

By definition, the nearest-neighbor (NN) occupied sites are said to be in the same cluster; two sites which are not nearest neighbor to each other but are connected by a sequence of NN occupied sites are said to be in the same cluster. A site whose neighbors are all vacant is a one-site cluster. When  $P_s$  is increased from small values to large-values, there is also a percolation transition at a critical probability  $P_{s,c}$ . In Fig. 2, some typical subgraphs without or with the percolating cluster are shown.

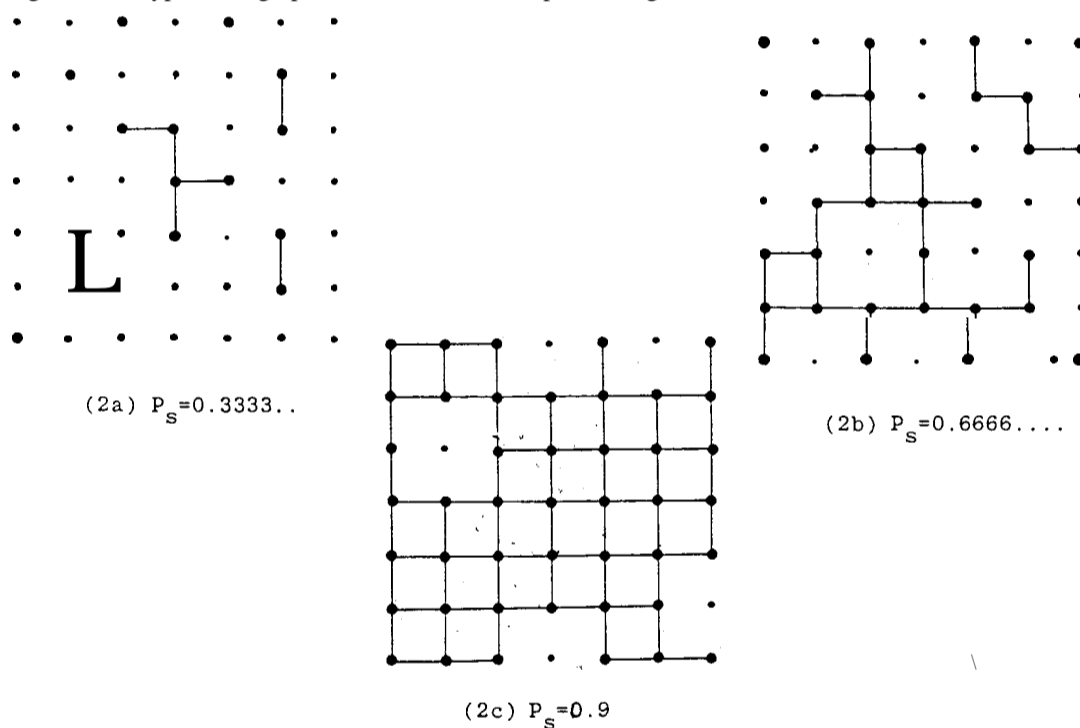


Fig. 2 Site percolation on a square lattice  $G$ . The site probabilities  $P_s$  for Fig. 2a, 2b, and 2c are 0.333 ..., 0.666. ., and 0.9, respectively. The occupied sites are represented by solid dots ( $\bullet$ ). The nearest-neighbor (NN) pairs of occupied sites are connected by solid lines ( $-$ ) and said to be in the same cluster.

In the site-bond random percolation on  $G$ , each site of  $G$  is occupied with the probability  $P_s$ . This process generates section graphs  $G^+ \subseteq G$ . Attaching a bond to every pair of the NN occupied sites in  $G^+$ , we obtain a subgraph  $G^* \subseteq G$  whose total number of attached bonds is  $u(G^+)$ . Now every bond of  $G^*$  is attached with a bond probability  $P_b$ . This process generates subgraphs  $G' \subseteq G^*$ . The probability weight for a given subgraph  $G'$  of  $v(G^+)$  occupied sites and  $b(G')$  attached bonds is given by:

$$\pi(G', P_s, P_b) = P_s^{v(G^+)} (1 - P_s)^{N - v(G^+)} P_b^{b(G')} \times (1 - P_b)^{u(G^+) - b(G')} \quad (2.3)$$

By definition, the occupied sites which are connected by a sequence of attached bonds and occupied sites are said to be in the same cluster. For small values of  $P_s$  and/or  $P_b$ , the dominant subgraphs contain only small clusters; for large values of  $P_s$  and  $P_b$ , the dominant subgraphs contain the percolating clusters. Examples of both cases are shown in Fig. 3. We may draw a phase boundary in the  $P_s - P_b$  plane to divide the plane into F-region and P-region as shown in Fig. 4 such that the systems of the F-region do

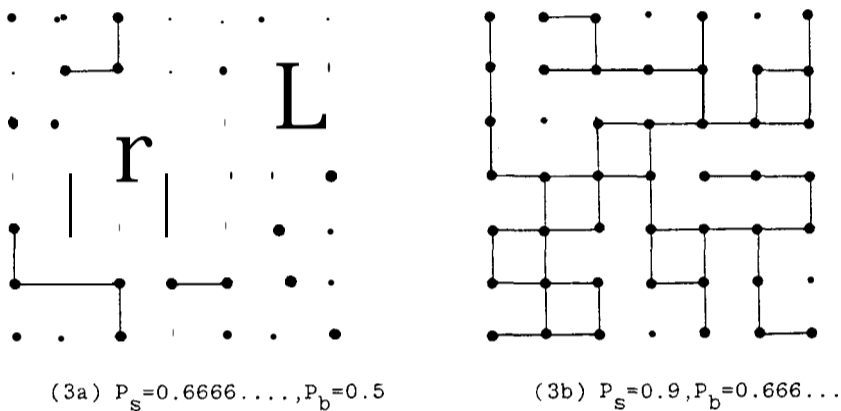


Fig. 3 Site-bond percolation on a square lattice with the site probability  $P_s$  and the bond probability  $P_b$ . In Fig. 3a,  $P_s = 0.6666\dots$ ,  $P_b = 0.5$ ; in Fig. 3b,  $P_s = 0.9$ ,  $P_b = 0.6666\dots$ . The occupied sites are connected by solid lines (—) with the bond probability  $P_b$ . The occupied sites connected by a sequence of solid lines and solid dots are said to be in the same cluster.

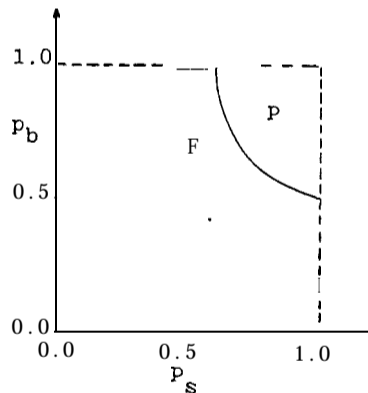


Fig. 4 Schematic phase diagram of the site-bond percolation on a square lattice. The solid curve is the phase boundary between the F-region and the P-region.

not have percolating clusters and the systems of the P- region have percolating clusters: When we increase  $P_s$  and/or  $P_b$  such that the  $(P_s, P_b)$  point moves from F-region to P-region, there is a percolation transition at the phase boundary. The site-bond random percolation contains the site random percolation as a special case when  $P_b = 1$  and  $0 \leq P_s \leq 1$  and contain the bond random percolation as a special case when  $P_s = 1$  and  $0 \leq P_b \leq 1$ . Unless specified otherwise, in this section we will consider site-bond percolation for further discussion.

If besides the factors on the right-hand side of Eq. (2.3), we include a  $G'$ -dependent factor  $g(G')$ , called correlation factor, in the probability weight for the subgraph  $G'$ ;

$$\pi_c(G', P_s, P_b) = \pi(G', P_s, P_b) g(G'), \quad (2.4)$$

then we have the correlated percolation model. An example of  $g(G')$  is

$$g(G') = q^{n_f(G')} \quad (2.5)$$

where  $n_f(G')$  is the number of nonpercolating clusters in  $G'$ . When  $q > 1$ , the system favors subgraphs with larger number of nonpercolating clusters. An example is given in Fig. 5. When  $g(G')$  is a constant independent of  $G'$ , the correlated percolation problem defined by Eq. (2.4) reduces to the random percolation problem.

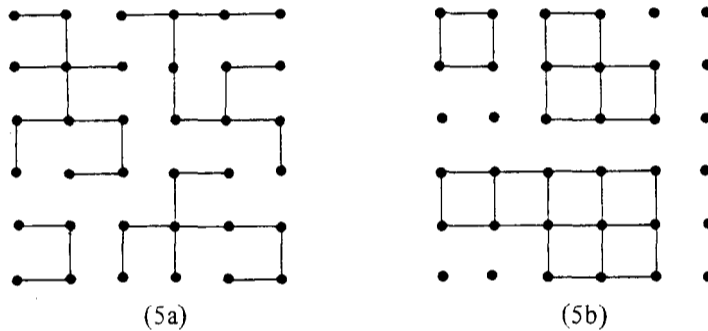


Fig. 5 Two subgraphs of the bond correlated percolation process on a square lattice with the correlation factor given by Eq. (2.5). Both subgraphs have 32 attached bonds, but Fig. 5a has 4 finite clusters and Fig. 5b has 14 finite clusters. If  $q < 1$ , Fig. 5a which has more ramified clusters, has larger probability weight; if  $q > 1$ , Fig. 5b, which has more compact clusters, has larger probability weight.

Based on the concept of clusters defined in the percolation problem, we may define some geometrical quantities. Let  $Q(G')$  be a  $G'$ -dependent geometrical quantity. We will use  $\overline{Q(G')}$  to represent the average of  $Q(G')$  over all subgraphs, and use  $\langle Q(G') \rangle_0$  to represent  $\overline{Q(G')}/N$  in the thermodynamic limit, i.e.

$$\overline{Q(G')} = \frac{\sum_{G' \subseteq G} \pi_c(G', P_s, P_b) Q(G')}{\sum_{G' \subseteq G} \pi_c(G', P_s, P_b)}, \quad (2.6)$$

$$\begin{aligned} \langle Q(G') \rangle_{\circ} &= \lim_{N \rightarrow \infty} Q(G')/N \\ &= \lim_{N \rightarrow \infty} \frac{\sum_{G' \subseteq G} \pi_c(G', P_s, P_b) Q(G')/N}{\sum_{G' \subseteq G} \pi_c(G', P_s, P_b)}. \end{aligned} \quad (2.7)$$

If  $Q(G')$  represent the total number of sites in percolating clusters,  $N^*(G')$ , then  $\langle Q(G') \rangle_{\circ}$  is the percolating probability  $P(G, P_s, P_b)$ , i.e. the probability that a site belongs to a percolating cluster. If  $Q(G')$  represents  $\sum_c n_c^2(G')$ , where the sum is over all non-percolating cluster  $c$  in  $G'$ , and  $n_c(G')$  is the number of sites in cluster  $c$ , then  $\langle Q(G') \rangle_{\circ}$  is the mean cluster size  $S(G, P_s, P_b)$ . If  $Q(G')$  represents  $[\delta b(G')]^2 = [b(G') - \bar{b}(G')]^2/N$ , then  $\langle Q(G') \rangle_{\circ}$  is the fluctuations of the number of bonds  $F(G, P_s, P_b)$ . Now we define a function:

$$\gamma_{ab}(G') = \begin{cases} 1 & \text{if site a and b are in the same cluster of } G' \\ 0 & \text{otherwise.} \end{cases}$$

The average  $\overline{\gamma_{ab}(G')}$  is the pair connectedness function  $P_{ab}(G, P_s, P_b)$ . In the limit  $N \rightarrow \infty$ , when the system is not at the percolation transition point and when the separation  $r$  between site  $a$  and site  $b$  is a large number, we expect:

$$\begin{aligned} P_{ab}(G, P_s, P_b) &\propto r^{-c} \exp[-r/\xi(G, P_s, P_b)] \\ &+ P^2(G, P_s, P_b), \end{aligned} \quad (2.8)$$

where  $c \geq 0$ . Eq. (2.8) defines the correlation length  $\xi(G, P_s, P_b)$ . At the percolation transition point, we expect:

$$P_{ab}(G, P_s, P_b) \propto r^{-(d-2+\eta_p)}, \quad (2.9)$$

which defines the exponent  $\eta_p$

Suppose  $P_s$  and  $P_b$  depend on a parameter  $\beta$  and when  $\beta$  increases from small values to large values, the point  $[P_s(\beta), P_b(\beta)]$  moves from the F-region of Fig. 4 to P-region of Fig. 4. The trajectory intersects the phase boundary at the point  $(P_{s,c}, P_{b,c})$  when  $\beta$  assumes the value  $\beta_c$ . Through many years of studies<sup>13</sup> after 1957, it was found that  $S(G, P_s, P_b)$ ,  $F(G, P_s, P_b)$ , and  $\xi(G, P_s, P_b)$  diverge at  $(P_{s,c}, P_{b,c})$  and  $P(G, P_s, P_b)$  increases rapidly from 0 to finite values when  $\beta$  increases from  $\beta_c$ . We may define critical exponents to characterize such behavior. When  $\beta$  increases from  $\beta < \beta_c$  to  $\beta_c$ , we have:

$$S(G, P_s, P_b) \sim |\beta - \beta_c|^{-\gamma_p} \quad (2.10)$$

$$F(G, P_s, P_b) \sim |\beta - \beta_c|^{-\alpha} P, \quad (2.11)$$

$$\xi(G, P_s, P_b) \sim |\beta - \beta_c|^{-\nu} P \quad (2.12)$$

When  $\beta$  increases from  $\beta_c$  to  $\beta > \beta_c$ , we have

$$S(G, P_s, P_b) \sim |\beta - \beta_c|^{-\gamma'} P, \quad (2.13)$$

$$F(G, P_s, P_b) \sim |\beta - \beta_c|^{-\alpha'} P, \quad (2.14)$$

$$\xi(G, P_s, P_b) \sim |\beta - \beta_c|^{-\nu'} P, \quad (2.15)$$

$$P(G, P_s, P_b) \sim |\beta - \beta_c|^{-\beta} P \quad (2.16)$$

For the pure bond and pure site percolation problems, we may simply take  $\beta = P_b$  and  $\beta = P_s$ , respectively, in Eqs. (2.10) to (3.16). It was found that the exponents defined in Eq. (2.9) to Eq. (2.16) have the universal property<sup>14</sup>, e.g. the bond percolation processes on square (SQ), plane triangular (PT), and honeycomb (HC) lattices have the same set of exponents. The exponents also satisfy certain scaling relations<sup>14</sup>, e.g.

$$\gamma' = \gamma \quad (2.17)$$

### III. PHASE TRANSITION IN THE POTTS MODEL

The behavior of the percolation transition considered in Section II is similar to the behavior of thermal phase transitions in Ising-like spin models. Here we take the q-state Potts model<sup>15</sup> as an example. In the q-state Potts model (QPM), each site of a lattice G of N sites and E bonds is occupied by a spin s with spin components  $-j, -(j-1), \dots, j$ , where  $2j+1=q$  and q is an integer. The Hamiltonian of the QPM may be written as:

$$H = -J \sum_{\langle ij \rangle} \delta(s_i, s_j) - h \sum_i s_i, \quad (3.1)$$

where the first and the second sums extend over all nearest-neighbor (NN) bonds and sites of G, respectively:  $\delta(s_i, s_j)$  equals 1 when  $s_i = s_j$  and equal 0 when  $s_i \neq s_j$ . The model of Eq. (3.1) corresponds the simple Ising model when  $q = 2$ . Note that the coupling of the external magnetic field h in Eq. (3.1) is different from that considered in Ref. 15, in which h couples only with one component of the Potts spin.

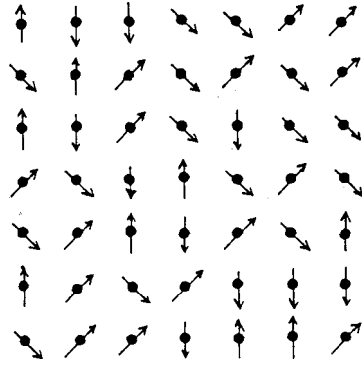


Fig. 6 The  $q$ -state Potts model defined on a  $6 \times 6$  square lattice with  $q$  being 4. At a given lattice site, there are four possible spin states:  $\uparrow$ ,  $\nearrow$ ,  $\searrow$ , and  $\downarrow$ . Two NN spins in the same direction will contribute  $-J$  to the total energy of the system.

The partition function  $Z(G, K, B)$  and the normalized free energy (by  $\beta = \frac{1}{kT}$ )  $f(G, K, B)$  of the QPM are defined by the equations:

$$Z(G, K, B) \equiv \sum_{s_1 \dots s_N} \exp[-\beta H], \quad (3.2)$$

$$f(G, K, B) \equiv \frac{1}{N} \ln Z(G, K, B), \quad (3.3)$$

where  $K = \beta J$  and  $B = \beta h$ .

Using  $f$  of Eq. (3.3), we may calculate the spontaneous magnetization  $M$ , zero-field magnetic susceptibility  $\chi$ , internal energy  $U$ , and the zero-field specific heat  $C_h$  of the QPM. They are:

$$M = \lim_{B \rightarrow 0^+} \lim_{N \rightarrow \infty} \frac{\partial}{\partial B} f(G, K, B), \quad (3.4)$$

$$\chi = \lim_{B \rightarrow 0^+} \lim_{N \rightarrow \infty} \beta \frac{\partial^2}{\partial B^2} f(G, K, B), \quad (3.5)$$

$$U = \lim_{B \rightarrow 0^+} \lim_{N \rightarrow \infty} \frac{-\partial}{\partial \beta} f(G, K, B), \quad (3.6)$$

$$C_h = \frac{\partial}{\partial T} U. \quad (3.7)$$

The two-spin correlation function  $\langle s_a s_b \rangle$  for spins at site  $a$  and site  $b$  of  $G$  is defined by the equation:



$$\langle s_a s_b \rangle = \frac{1}{Z(G, K, B)} \sum_{s_1 \dots s_N} \exp[-\beta H] s_a s_b . \quad (3.8)$$

It was found<sup>14</sup> that for given space dimensions  $d$ , there exists a critical spin component  $q_c(d)$  so that the phase transition is second order for  $q \leq q_c$  and the phase transition is first order for  $q > q_c$ . In the former case, and for a large separation  $r$  between site  $a$  and site  $b$ , we expect that

$$\langle s_a s_b \rangle \sim r^{-c} \exp[-r/\xi(G, T)] + M^2 \quad (3.9)$$

with  $c \geq 0$  when  $T \neq T_c$  and

$$\langle s_a s_b \rangle \sim r^{-(d-2+\eta)} \quad (3.10)$$

when  $T = T_c$ . Eq. (3.9) and (3.10) define the correlation length  $\xi(G, T)$  and the critical exponent  $\eta$ , respectively. We may define other critical exponents to characterize the behavior of physical quantities near the critical point  $\beta_c = \frac{1}{kT_c}$ . When  $T \rightarrow T_c^+$ , we have:

$$\chi \sim (T - T_c)^{-\gamma} , \quad (3.11)$$

$$C_h \sim (T - T_c)^{-\alpha} , \quad (3.12)$$

$$\xi \sim (T - T_c)^{-\nu} . \quad (3.13)$$

When  $T \rightarrow T_c^-$ , we have

$$\chi \sim (T_c - T)^{-\gamma'} , \quad (3.14)$$

$$C_h \sim (T_c - T)^{-\alpha'} , \quad (3.15)$$

$$M \sim (T_c - T)^\beta , \quad (3.16)$$

$$\xi \sim (T_c - T)^{-\nu'} . \quad (3.17)$$

It was found that the exponents defined in Eq. (3.10) to (3.17) have the universal property<sup>15</sup>, e.g., the SQ lattice QPM, PT lattice QPM, and the HC lattice QPM have the same set of critical exponent for a given  $q \leq q_c$ . The exponents also satisfy certain scaling relations", e.g.

$$\gamma' = \gamma , \quad (3.18)$$

$$\alpha + 2\beta + \gamma' = 2. \quad (3.19)$$

It was also found<sup>15</sup> that  $\alpha$  increases with  $q$

#### IV. PERCOLATION TRANSITION AND THERMAL PHASE TRANSITIONS

The percolation transition considered in Section II and the thermal phase transition considered in

Section III have similar behavior. Since 1974, many scientists have tried to answer the question<sup>16</sup>: "Whether the phase transition in the Ising model is a percolation transition?" To answer this question, one must unambiguously define clusters for the Ising system such that at high temperatures, the system has only small nonpercolating clusters. And at low temperatures the system has at least one percolating cluster. When the temperature is decreased from high temperatures to low temperatures, there is a percolation transition at a temperature  $T_p$ . As in the case of the percolation considered in Section II, one may also define the percolation probability,  $P$ , the mean cluster size  $S$ , pair connectedness function and the corresponding correlation length  $\xi$ , etc. for the clusters of the Ising model. If the phase transition of the Ising model is a percolation transition, then  $T_p = T_c$  and the critical exponents ( $\beta_p, \gamma_p, \gamma'_p, \nu_p, \nu'_p, \eta_p$  etc) of the clusters are the same as the corresponding Ising critical exponents ( $\beta, \gamma, \gamma', \nu, \nu', \eta$ , etc).

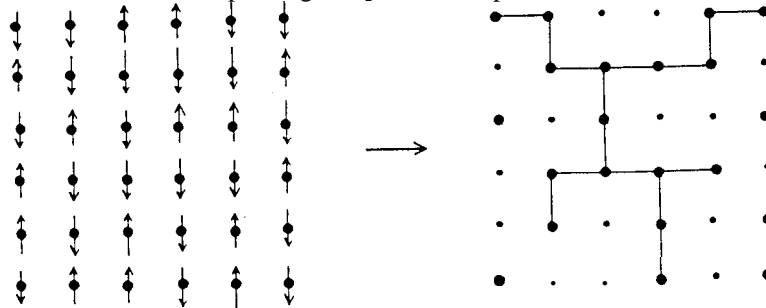


Fig. 7 Fisher's idea of mapping from the Ising system to a cluster or site correlated percolation model. The down spins ( $\downarrow$ ) and the up spins ( $\uparrow$ ) are mapped into occupied sites ( $\bullet$ ) and vacant sites ( $\cdot$ ), respectively. Two NN occupied sites are always in the same cluster and connected by a solid line.

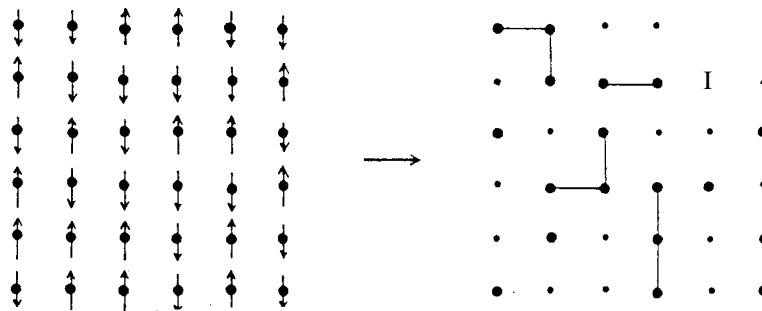


Fig. 8 Coniglio and Klein's idea of mapping from the Ising system to a site-bond correlated percolation model. The down spins ( $\downarrow$ ) and the up spins ( $\uparrow$ ) are mapped into occupied sites ( $\bullet$ ) and vacant sites ( $\cdot$ ), respectively. Two NN occupied sites are in the same cluster with a bond probability  $P_b$  introduced artificially.

Traditionally, researchers followed Fisher's idea<sup>17</sup> and considered the lattice sites with an Ising spin  $\sigma = -1$  occupied and the lattice sites with an Ising spin  $\sigma = +1$  unoccupied: the nearest neighbor (NN) occupied sites were considered to be in the same cluster. The ferromagnetic interactions between Ising spins makes the occupation of lattice sites correlated and the Ising model is thus mapped into a site correlated percolation model (SCPM). It was found<sup>16</sup> that for the two dimensional lattice  $T_p = T_c$  but  $\gamma_p = 1.91 > \gamma = 1.75$  and for the three dimensional lattice  $T_p \neq T_c$ . The results  $\gamma_p = 1.91 > \gamma = 1.75$  indicates that the mean cluster size of the SCPM grows too faster when  $T \rightarrow T_c$ . To make the mean cluster size grow slowly, Coniglio and Klein<sup>18</sup> considered that the occupied sites defined above were in the same cluster with a probability  $P_b$ . The Ising model was thus mapped into a site-bond correlated percolation

model (SBCPM). Coniglio and Klein<sup>18</sup> found that for  $P_b = 1 - \exp(-K)$ , where  $K = J/kT$  is the normalized NN coupling constant for the Ising model,  $T_p = T_c$ ,  $\nu_p = \nu$ , and  $\gamma_p = 7$ . However, in this SBCPM<sup>19</sup> "the bonds are only introduced to define the connectivity between two nearest-neighbor particles and do not affect their interacting energy and therefore the particle distribution." Therefore Coniglio and Klein only defined a SBCPM which has the same critical property the Ising model, but they did not prove that the phase transition of the Ising model is a percolation transition.

In recent papers<sup>8-12</sup>, Hu proposed that in establishing the connection between the Ising-like spin models and correlated percolation models, one should consider the sites with a spin occupied and only the sites without a spin unoccupied. One should also consider the two-spin coupling as a bond with a bond probability  $P_b$  depending on the coupling strength  $J$  and the temperature  $T$ . An example of such a mapping is shown in Fig. 9. In the  $q$ -state Potts model (QPM) of Eq. (3.1), every lattice site is occupied by a Potts spin  $s$ . It is easy to show that the QPM may be mapped into the  $q$ -state bond-correlated percolation model (QBCPM).

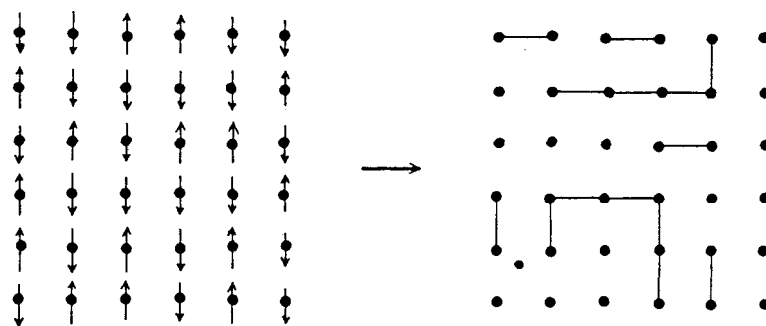


Fig. 9 Hu' s idea of mapping from the Ising system to a correlated percolation model. All lattice sites with a spin are considered occupied ( $\bullet$ ) in disregard of the directions of the spins. Two NN occupied sites are in the same cluster with a bond probability  $P_b$  determined by the coupling constant and the temperature of the system.

The partition function of the QPM may be written as:

$$\begin{aligned} Z(\mathbf{G}, K, B) &= \sum_{s_1 \dots s_N} \exp \left[ K \sum_{\langle ij \rangle} \delta(s_i, s_j) \right] \prod_1 \exp(Bs_i) \\ &= \sum_{s \dots s_N} \prod_{\langle ij \rangle} \left[ 1 + (e^K - 1) \delta(s_i, s_j) \right] \prod_1 \exp(Bs_i) \end{aligned} \quad (4.1)$$

Now we expand the first product in Eq. (4.1) and use the subgraphs  $G' \subseteq G$  to represent the terms in the expansion. A subgraph  $G'$  of a 6x6 square lattice is shown in Fig. 10 as an illustration. For each NN pair of sites  $\langle ij \rangle$  there occurs in Eq. (4.1) the two terms: 1 and  $[\exp(2K) - 1] \delta(s_i, s_j)$ ; subgraph  $G'$  with no  $\langle ij \rangle$  bond correspond to the former and those with an  $\langle ij \rangle$  bond to the latter. There are  $b(G')$  bonds in the subgraph  $G'$ ,  $0 \leq b(G') \leq E$ . The clusters are defined in the same way as the bond percolation of Section II. After sum over spin states, we have

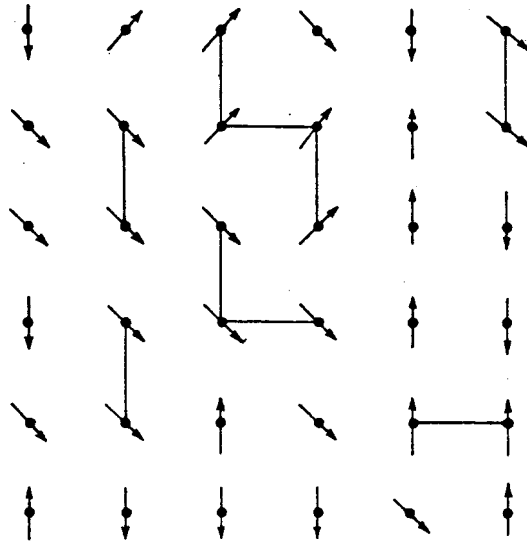


Fig. 10 A subgraph  $G'$  of a  $6 \times 6$  square lattice  $G$  and a spin state on  $G$ . The solid lines represent bonds in the  $G'$ . At a given lattice site, there are four possible spin states:  $\uparrow, \nearrow, \searrow$  and  $\downarrow$ , i.e.  $q = 4$ . Note that the spins connected by bonds must be in the same spin state.

$$\begin{aligned}
 Z(G, K, B) &= \sum_{G' \subseteq G} (e^K - 1)^{b(G')} \pi_c [ \exp(Bn_c j) + \exp(Bn_c(j-1)) \\
 &\quad + \dots + \exp(-Bn_c j) ] \\
 &= e^{KE} \sum_{G' \subseteq G} P_b^{b(G')} (1 - P_b)^{E-b(G')} \pi_c [ \exp(Bn_c j) \\
 &\quad + \exp(Bn_c(j-1)) + \dots + \exp(-Bn_c j) ],
 \end{aligned} \tag{4.2}$$

where the product extends over all cluster  $c$  in  $G'$ .  $n_c \equiv n_c(G')$  is the number of sites in the cluster  $c$ , and

$$P_b = 1 - e^{-K} \tag{4.3}$$

With the notations of Eqs. (2.6) and (2.7) and with  $Z(G, K, B)$  of Eq.(4.2) in Eq.(3.3), it follows from Eqs. (3.4) to (3.7) that:

$$\begin{aligned}
 M &= \lim_{N \rightarrow \infty} W^{-1} \sum_{G' \subseteq G} \pi(G', P_b, q) [N^*(G') / N] j \\
 &\equiv j \langle N^*(G') \rangle_0,
 \end{aligned} \tag{4.4}$$

$$\chi = A \left\langle \sum_c^f n_c^2(G') \right\rangle_0 + \lim_{N \rightarrow \infty} j^2 W^{-2} \sum_{G' \in \underline{CG}} \sum_G \pi(G', P_b, q) \times \pi(G'', P_b, q) [N^*(G') - N^*(G'')]^2 / (2N), \quad (4.5)$$

$$U = - \frac{J}{P_b} \langle b(G') \rangle_0, \quad (4.6)$$

$$C_h = \frac{kK}{P_b^2} [ - (1 - P_b) \langle b(G) \rangle_0 + \langle (\delta b(G'))^2 \rangle_0 ], \quad (4.7)$$

where

$$\pi(G, P_b, q) = P_b^{b(G')} (1 - P_b)^{E-b(G')} q^{n_f(G')}, \quad (4.8)$$

$$W = \sum_{G' \in \underline{CG}} \pi(G, P_b, q), \quad (4.9)$$

$$A = [j^2 + (j-1)^2 \mathbf{t} \dots \mathbf{t} (-j+1)^2 \mathbf{t} (-j)^2] = \frac{1}{12} (q^2 - 1), \quad (4.10)$$

$$\delta b(G') = b(G') - b(G''). \quad (4.11)$$

$N^*(G')$  of Eqs. (4.4) and (4.5) is the total number of sites in the percolating clusters in  $G'$ ,  $n_f(G')$  of Eq. (4.8) is the total number of nonpercolating clusters in  $G'$ .  $\sum_c^f$  of Eq. (4.5) is a sum over all nonpercolating clusters in  $G'$ . From Eq. (4.4) to Eq. (4.11), it is obvious that  $Z(G, K, B)$  of Eq. (4.2) is the generating function of the  $q$ -state bond-correlated percolation model (QBCPM) with the bond probability  $P_b$  and the correlation factor given by Eq. (4.3) and

$$g(G') = q^{n_f(G')}, \quad (4.12)$$

respectively.

The percolation probability, mean cluster size, and fluctuations of the number of bonds of the QBCPM are related to the spontaneous magnetization, magnetic susceptibility, and specific heat, respectively, of the QPM. Therefore  $\beta_p = \beta$ ,  $\gamma_p = \gamma$ ,  $\alpha_p = \alpha$ , and  $\alpha'_p = \alpha'$  when  $q \leq q_c$ . If the second term in Eq. (4.5) is not more singular than the first term, then  $\gamma'_p = \gamma$  when  $q \leq q_c$ . Eq. (3.8) may be written as:

$$\langle s_a s_b \rangle = \frac{1}{Z(G, K, B) s_1 \dots s_N} \sum_{\langle ij \rangle} \pi [1 + (e^K - 1) \delta(s_i, s_j) - 1 s_a s_b \pi \exp(Bs_i)] \quad (4.13)$$

Using a procedure similar to that used to derive Eq. (4.2), we expand the first product in Eq. (4.13) and use the subgraphs  $G' \subseteq G$  to represent the terms in the expansion. Carrying out the summation over spin states, we can show that  $\langle s_a s_b \rangle$  in the thermodynamic limit and at  $B = 0^+$ , denoted by  $\Gamma(s_a, s_b)$ , can be written as:

$$\Gamma(s_a, s_b) = \lim_{N \rightarrow \infty} W^{-1} \sum_{G' \subseteq G} \pi(G', P_b, q) \gamma_{ab}(G') f(q), \quad (4.14)$$

where  $\gamma_{ab}(G')$  is defined in Section II,  $f(q)$  equals 1 when  $q$  is an even integer and equals  $(q-1)/q$  when  $q$  is an odd integer. The right-hand side of Eq. (4.14) is just the pair connectedness function of the sites  $a$  and  $b$  in the QBCPM. Therefore when  $q \leq q_c$  the critical exponents  $\nu_p, \nu_p'$ , and  $\eta_p$  of the QBCPM equal  $\nu, \nu'$  and  $\eta$  of the QPM, respectively. Therefore, the clusters in the QBCPM have the same critical point and order of phase transition as the QPM. When  $q \leq q_c$ , their critical exponents  $\beta_p, \gamma_p$  (perhaps also  $\gamma_p'$ ),  $\alpha_p, \alpha_p', \nu_p, \nu_p'$  and  $\eta_p$  are the same as the corresponding values for the QPM.

Using the connection between the QPM and QBCPM, we may establish a geometrical condition of the phase transition in the QPM. Eq. (4.4) indicates that for  $P_b < P_{b,c} \equiv 1 - \exp(-J/kT_c)$ , subgraphs without percolating clusters, denoted by  $G_f'$ , dominate the contribution to the summation (over all subgraphs) and for  $P_b > P_{b,c}$  subgraphs with percolating clusters: denoted by  $G_p'$ , dominate the contribution to the summation. Now we consider the following partial sums over subgraphs  $G_f'$  and  $G_p'$ , respectively :

$$W_f = e^{KE} \sum_{G_f' \subseteq G} \pi(G_f', P_b, q), \quad (4.15)$$

$$W_p = e^{KE} \sum_{G_p' \subseteq G} \pi(G_p', P_b, q). \quad (4.16)$$

For  $P_b < P_{b,c}$ ,

$$W_p < W_f, \quad (4.17)$$

for  $P_b > P_{b,c}$

$$W_p > W_f, \quad (4.18)$$

and at  $P_c$  we expect

$$W_f = W_p, \quad (4.19)$$

which is the geometrical condition of phase transition.  $W_f$  may be rewritten as:

$$\begin{aligned} W_f &= \sum_{G_f' \subseteq G} (e^K - 1)^{b(G')} q^{n_f(G_f')} \\ &= \sum_{R=0}^E U(K)^R E g_f(q, R) \end{aligned} \quad (4.20)$$

where

$$U(K) = e^K - 1, \quad (4.21)$$

$$0 \leq R \equiv b(G') / E \leq 1, \quad (4.22)$$

$$g_f(q, R) = \sum_{G_f' \subseteq G} q^{n_f(G_f')}. \quad (4.23)$$

The sum in Eq. (4.23) is over all  $G_f'$  with a fixed fraction  $R$  of occupied bonds. In the large  $E$  limit, the sum in Eq. (4.20) may be represented by an integration, i.e.

$$W_f = E \int_0^1 U(K)^{RE} g_f(q, R) dR \quad (4.24)$$

Similarly, in the large  $E$  limit,  $W_p$  of Eq. (4.16) may be written as:

$$W_p = E \int_0^1 U(K)^{RE} g_p(q, R) dR, \quad (4.25)$$

with  $g_p(q, R)$  given by:

$$g_p(q, R) = \sum_{G_p' \subseteq G} q^{n_p(G_p')}, \quad (4.26)$$

where the sum is over all  $G_p'$  with a fixed fraction  $R$  of occupied bonds. It is clear that the dependence of  $W_f$  and  $W_p$  on the coupling constant  $J$  and the temperature  $T$  comes only from the factor  $U(K)^{RE}$ . In the following, we will call  $U(K)^{RE}$  "the interaction factor" and call  $g_f(q, R)$  and  $g_p(q, R)$  "the geometrical factor".

For a fixed  $K$  and a fixed large  $E$ ,  $U^{RE}$  is a monotonous function of  $R$ , but  $g_f(q, R)$  and  $g_p(q, R)$  are expected to peak sharply at certain values, say  $R_f$  and  $R_p$ , respectively. It is reasonably to expect that the integrands in Eqs. (4.24) and (4.25) also peak sharply at certain values, say  $\bar{R}_f$  and  $\bar{R}_p$ , respectively. Expanding the logarithm of the integrands of Eq. (4.24) and (4.25) at  $\bar{R}_f$  and  $\bar{R}_p$ , respectively and keeping only the leading and the quadratic terms, we have:

$$W_f \cong EU(K)^{E\bar{R}_f} g_f(q, \bar{R}_f) \int_0^1 \exp \left[ -\frac{1}{2} \Gamma_f (R - \bar{R}_f)^2 \right] dR \equiv W_f^*, \quad (4.27)$$

$$W_p \cong EU(K)^{E\bar{R}_p} g_p(q, \bar{R}_p) \int_0^1 \exp \left[ -\frac{1}{2} \Gamma_p (R - \bar{R}_p)^2 \right] dR \equiv W_p^*, \quad (4.28)$$

where

$$\Gamma_f = - \left[ \frac{\delta^2}{\delta R^2} \ln [U(K)^{RE} g_f(q, R)] \right]_{\bar{R}_f}, \quad (4.29)$$

$$\Gamma_p = - \left[ \frac{\delta^2}{\delta R^2} \ln [U(K)^{RE} g_p(q, R)] \right]_{\bar{R}_p}, \quad (4.30)$$

In the approximation of Eq. (4.27) and (4.28), the geometrical condition of phase transition at  $T_c$  is given by:

$$W_f^* = W_p^* \quad (4.31)$$

Using notations of Eq. (4.24) and (4.25), the average number of occupied bonds  $\overline{b(G')}$  may be written as:

$$\overline{b(G')} = W^{-1} E \left[ \int_0^1 U(K)^{RE} g_f(q, R) R dR + \int_0^1 U(K)^{RE} g_p(q, R) R dR \right] \quad (4.32)$$

Since " $R$ " in the integrand of Eq. (4.32) changes much slowly than  $U^{RE} g_f$  and  $U^{RE} g_p$  with  $R$ , we may use the approximation of Eqs. (4.27) and (4.28) to rewrite Eq. (4.32) as:

$$\overline{b(G')} = (W_f^* b_f + W_p^* b_p) / (W_f^* + W_p^*), \quad (4.33)$$

where

$$b_f = \overline{R}_f E, \quad (4.34)$$

$$b_p = \overline{R}_p E \quad (4.35)$$

For  $T > T_c$ ,  $W_f^* \gg W_p^*$  and we have

$$\overline{b(G')} = b_f; \quad (4.36)$$

for  $T < T_c$ ,  $W_f^* \ll W_p^*$  and we have

$$\overline{b(G')} = b_p; \quad (4.37)$$

for  $T = T_c$ ,  $W_f^* = W_p^*$  and we have

$$\overline{b(G')} = \frac{1}{2} (b_f + b_p) \quad (4.38)$$

For systems with  $d \geq 2$ , it is difficult to calculate exactly  $g_f(q, R)$  and  $g_p(q, R)$ . However, for the one dimensional systems, we<sup>20</sup> are able to write down an exact formula for  $g_f(q, R)$ . We find that in this system Eq. (4.36) is indeed satisfied.

For a large but finite system with  $N$  spins, the internal energy is given by:

$$U = \frac{-J}{P_b} \overline{b(G')} / N. \quad (4.39)$$

It follows from Eq. (4.7) that the specific heat  $C_h$  of the QPM contains a term proportional to the internal energy  $U$  and a term proportional to the fluctuations of the number of bonds  $\langle [\delta b(G')]^2 \rangle$ . It is clear that the divergence of  $C_h$  at  $T_c$  comes from the contribution of the latter. For  $T \gg T_c$  ( $T \ll T_c$ ),  $W_f \gg W_p$  ( $W_f \ll W_p$ ) and we expect that  $\langle [\delta b(G')]^2 \rangle$  is determined by  $\Gamma_f(\Gamma_p)$ . At  $T_c$ ,



both peaks at  $R_f$  and  $R_p$  are important and we expect that the leading term of the specific heat is given by:

$$\begin{aligned} Ch^* &= \frac{kK^2}{P_b^2} \langle [\delta b(G')]^2 \rangle \\ &\cong \frac{kK^2}{P_b^2} \frac{W_f^* [b_f - \overline{b(G')}]^2 + W_p^* [b_p - \overline{b(G')}]^2}{(W_f^* + W_p^*) N} \\ &= \frac{kK^2}{P_b^2} \frac{(b_p - b_f)^2}{4N} \end{aligned} \quad (4.40)$$

where Eq. (4.31) and Eq. (4.33) have been used. Assuming that at the phase transition point

$$b_p - b_f = b_0 N^a, \quad (4.41)$$

where  $b_0$  and  $a$  are constants and  $0 < a \leq 1$ , we have:

$$C_h^* = \frac{kK^2}{4P_b^2} b_0^2 N^{2a-1} \quad (4.42)$$

However, from the finite-size scaling of the specific heat at second-order phase transitions<sup>21</sup>, we have

$$C_h^* \sim N^\alpha / (2-\alpha) \quad (4.43)$$

Comparing Eq. (4.42) and (4.43), we have

$$\alpha = (2a - 1) / a = 2 - \frac{1}{a}, \quad (4.44)$$

which shows that  $\alpha$  increases with  $a$ .

It follows from Eq. (4.8) that the subgraphs with larger number of finite clusters increase their relative probability weight when  $q$  is increased. For a given  $R < 1$ , especially  $R \ll 1$ , we expect that the subgraphs  $G_f$  contributing to the summation of Eq. (4.23) are usually more compact, hence have more closed loops and finite clusters (Euler relations), than the subgraphs contributing to the summation of Eq. (4.26). Therefore when  $q$  is increased  $W_f$  will increase faster than  $W_p$  and that  $R_f$  will move toward smaller values of  $R$  with a speed faster than that of  $R_p$ . After increasing  $q$  to a new value, we must also increase  $K$  to a new value so that Eq. (4.19) or Eq. (4.31) may still be true. At the new  $K$ , the separation between  $R_p$  and  $R_f$  is expected to increase, i.e.  $a$  of Eq. (4.41) will increase with  $q$ . It follows from Eq. (4.44) that  $\alpha$  will increase with  $q$ . When  $q$  is larger than a critical value  $q_c$ ,  $a$  of Eq. (4.41) will assume its largest value 1 and we have

$$b_p - b_f = b_0 N, \quad (4.45)$$

$$C_h^* = \frac{kK^2}{4P_b^2} b_0 N = \frac{\ell^2}{4kT_c^2} N, \quad (4.46)$$

$$\ell = U^+ - U^- = \frac{J}{z} b_0, \quad (4.47)$$

where  $U^+$  and  $U^-$  are internal energies at  $T_c + \epsilon$  and  $T_c - \epsilon$ , respectively with  $\epsilon$  being an infinitesimal positive number. Thus for  $q > q^*$ , the latent heat  $\ell > 0$  and the phase transition is first-order. We may identify  $q^*$  with  $q_c$  mentioned Section III. Eq. (4.46) is the finite-size scaling of specific heat at a first-order phase transition<sup>21</sup>. The finite-size rounding of the transition temperature  $T_c$  at a first-order phase transition may be estimated from the equation<sup>21</sup>:

$$C \sim \frac{\ell}{\Delta T_c} \quad (4.48)$$

It follows from Eq. (4.46) and (4.48) that

$$\frac{\Delta T_c}{T_c} \sim \frac{kT}{N\ell} \equiv \frac{1}{N\sigma} \quad (4.49)$$

which is consistent with the result proposed by Imry<sup>22</sup>.

In conclusion, we have shown that the phase transition in the QPM corresponds the percolation transition of a QBCPM. Using the geometrical condition of the phase transition based on such a connection, we have given the geometrical interpretation of the increase of  $\alpha$  with  $q$  for  $q \leq q_c$ , changeover from second-order to first-order phase transition as  $q$  increases, finite size scaling of specific heat and the rounding of transition temperature at a first-order phase transition.

## V. EXTENSION TO OTHER SYSTEMS

The method of Section VI may be applied to other lattice interacting systems. Here we briefly mentioned some of the result.

- A. A sublattice-dilute  $q$ -state Potts model (SDQPM) has been mapped<sup>9</sup> into a sublattice-dilute  $q$ -state site-bond-correlated percolation model (SDQSBCPM)<sup>23</sup> and a dilute  $q$ -state Potts model (DQPM)<sup>24</sup> has been mapped<sup>9</sup> into a  $q$ -state site-bond-correlated percolation model (QSBCPM).
- B. The Ising model with multi-spin interactions, e.g. the Baxter model<sup>26</sup>, has been mapped<sup>27</sup> into the multisite correlated percolation model in which the active element in the random process may involve more than two sites.

For each spin model considered in subsection V.A and V.B, the phase transition is just the percolation transition of the corresponding percolation model. From this connection, we may write down a geometrical condition of phase transitions similar to Eq. (4.19). We may also introduce the interaction factor and the geometrical factors to analyze the behavior of the system. For the model of subsection V.A, the geometrical factor should depend on the fraction of occupied sites  $R_s$  and the fraction of occupied bonds  $R_b$ . For the model of subsection V.B, the geometrical factor should depend on the fraction of multisite active elements  $R_m$  and the fraction of occupied bonds  $R_2$ . Therefore the analysis is more complicated.

- C. We have written an interaction Hamiltonian for the hydrogen bonding in water molecules *on a lattice* and shown that the partition function for this interaction Hamiltonian may be expressed as the generating function of a bond-correlated percolation model with a bond probability depending on the hydrogen-bond strength  $J$  and the temperature  $T$ . This percolation model of the hydrogen bonding can be used to explain some peculiar behavior of supercooled water. In this model certain assumptions made in Stanley and his coworker's model<sup>28</sup> of supercooled water do not present but could be derived directly from the theory.
- D. We have formulated a percolation theory of reversible sol-gel phase transitions in solvent<sup>12</sup> which do not have certain phenomenological parameter introduced in Coniglio, Stanley and Klein's theory<sup>29</sup>

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