

## **Renormalization Group Approach for the Site-Bond Percolation in Structured Stochastic Environments**

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The quenched averaged percolation problem of a lattice with a given structure is analyzed. The structure is described by the static structure factor  $S(q) \sim q^{-a}$  in the region  $q \rightarrow 0$ . As a result of the renormalization group, it follows that the critical behavior for  $a < 2$  is the same as in the random percolation. In the case of  $a = 2$  second universality class with  $\eta = 0$  and  $\nu = 1/2 + \varepsilon/8 + \varepsilon^2/32$  is predicted.

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**KEY WORDS:** Renormalization group; percolation; disorder.

### **1. INTRODUCTION**

The formation of molecular networks (for instance, the formation of a gel starting from monomers) can be described in an obvious way by using the percolation concept. The classical percolation model is based on a lattice with translation symmetry, in which each lattice point is a monomer and each lattice site is a latent bond. In the network formation process this latent bond will be transformed into real bonds. Then, the occupation probability  $p$  is the measure of the formed bonds. Analytical<sup>(3,4)</sup> and numerical<sup>(8)</sup> investigations show the well-known critical behavior near the sol-gel transition. Many network formation processes realize structures where not all lattice points are occupied by a monomer. The simplest case is the random bond percolation on a dilute lattice.<sup>(1,9-11)</sup> Here, we have a random distribution of vacancies of the lattice, e.g., as a result of this dilution not all lattice sites are latent bonds (such a bond must be neighbor to two monomers). Now, the formation process is a percolation of a lattice with a quenched disorder. Against this percolation of a randomly diluted lattice, a more realistic situation is given by a spatial distribution of the

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monomers with a nonconstant probability function  $P$ , from which follows the well-defined static structure factor  $S(q)$  as a characteristic structure value. The determination of the critical behavior near the percolation threshold of such a system is the central aim of this paper.

## 2. MODEL AND RESULTS

We start our consideration from a quenched site dilute lattice, where the lattice sites are randomly occupied by Potts spins. The distribution of occupied sites is homogeneous and isotropic and may be characterized by a static structure factor  $S(|\mathbf{k}|)$ . The Potts Hamiltonian for this quenched site-diluted model reads<sup>(1,2)</sup>

$$H = -K \sum_{\langle ij \rangle} c_i c_j [\delta_{\sigma_i, \sigma_j} - 1] + \omega \sum_i [\delta_{\sigma_i, 1} - 1] \quad (1)$$

$\sigma_i = 1, \dots, s$  represents the Potts spin at the lattice point  $i$ ;  $c_i = 0, 1$  is the character of this lattice point ( $c_i = 0$ : vacancy). In percolation theory the constant  $K$  determines the bond probability  $p = 1 - e^{-K}$  and  $\omega$  represents an external field. The summation in the first part of Eq. (1) contains all pairs of neighboring lattice sites. From this Hamiltonian there follow in a well-known way<sup>(1)</sup> the characteristic values of the percolation theory, which in the case of a dilute lattice are a functional of the lattice structure. After averaging over the actual structure  $\mathbf{c}$  we get for the average number of clusters  $N_{Cl}$ , the average cluster mass  $P_{gel}$ , and the weight-average molecular weight  $M^{(2)}$  (all values per unit volume)

$$N_{Cl} = \langle F(\mathbf{c}, \omega) \rangle_{\mathbf{c}} \Big|_{\omega=0} + \bar{c} - 1 \quad (2)$$

$$P_{gel} = \frac{\partial}{\partial \omega} \langle F(\mathbf{c}, \omega) \rangle_{\mathbf{c}} \Big|_{\omega=0} + \bar{c} - 1 \quad (3)$$

$$M^{(2)} = \frac{\partial^2}{\partial \omega^2} \langle F(\mathbf{c}, \omega) \rangle_{\mathbf{c}} \Big|_{\omega=0} + \bar{c} - 1 \quad (4)$$

with the actual, structure-dependent free energy

$$F(\mathbf{c}, \omega) = \lim_{N \rightarrow \infty} \frac{\partial}{\partial S} \ln \sum_{\{\sigma\}} e^{-H} \quad (5)$$

and the concentration  $\bar{c}^+$  of occupied lattice sites.

Analogously, the quenched averaged pair connected  $P_{ij}$  can be obtained by introducing an inhomogeneous field  $\omega_i$  at each site  $i$ ,

$$P_{ij} = \frac{\partial^2}{\partial \omega_i \partial \omega_j} \langle F(\mathbf{c}, \omega) \rangle_{\mathbf{c}} \Big|_{\omega=0} \quad (6)$$

Writing the Potts spins states in (1) as a set of  $s$  vectors  $e_a^\alpha$  in  $(s-1)$ -dimensional space<sup>(3,4)</sup> ( $\alpha = 1, \dots, s$  and  $a = 1, \dots, s-1$ )

$$e_a^\alpha e_a^\beta = s\delta^{\alpha\beta} - 1$$

which reflects the full symmetry of the model, we find that the partition function  $Z$  becomes a functional integral by a typical transformation<sup>(5)</sup> in a continuous spin representation with the new field variables  $\Phi_i^a$  ( $a = 1, \dots, s-1, i = 1, \dots, N$ , lattice site,  $\omega = 0$ )

$$Z[\mathbf{c}] = \int D\Phi \exp \left[ -\frac{1}{2} \sum_{ij,a} \Phi_i^a M_{ij} \Phi_j^a + \sum_{i,a} V(c_i \Phi_i^a) \right] \tag{7}$$

with the structure-dependent potential

$$\begin{aligned} V(c_i \Phi_i^a) &= \ln \sum_{\{\alpha\}} \exp(c_i \Phi_i^a e_a^\alpha) \\ &= c_i \frac{1}{2} \Phi_i^2 - c_i \frac{1}{6} Q_{abc} \Phi_i^a \Phi_i^b \Phi_i^c - c_i \frac{1}{24} T_{abcd} \Phi_i^a \Phi_i^b \Phi_i^c \Phi_i^d \end{aligned} \tag{8}$$

Note that in this representation the identity  $c_i^2 = c_i$  was used. Using  $c_i = \bar{c} + \xi_i$  with  $\xi_i = 1 - \bar{c}, -\bar{c}$  and writing the tensor  $\mathbf{\Phi M \Phi}$  in terms of local values  $(\Phi^2, (\nabla\Phi)^2)$ , a simple diagram theory follows. From example, the two-point Green function  $G(q, \xi)$  becomes a diagram series, which is shown in Fig. 1. Each wavy line characterizes in this representation an external field  $\xi$ . The quenched average over this external field with the given probability  $P(\mathbf{c}, t)$  generates Fourier-transformed correlation functions  $\langle \xi_{q_1} \xi_{q_2} \dots \xi_{q_n} \rangle$  of the lattice structure. A simple algebraic investigation shows<sup>(6)</sup> that a separation of this function is possible with

$$\langle \xi_{q_1} \xi_{q_2} \dots \xi_{q_n} \rangle = C \sum_{\text{combinations}} \prod_{\text{pairs}} [S(q_i) \delta(\mathbf{q}_i - \mathbf{q}_j)] + o\left(\frac{1}{V}\right) \tag{9}$$

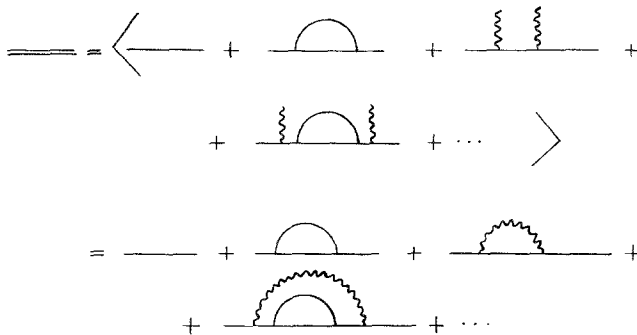


Fig. 1. Quenched average of the propagator  $G$ .

where  $S(q)$  is the static structure factor. Therefore, the quenched average over the diagrams produces the sum over all combinations of different pair connections between the  $\xi$  lines. The weight of such a structure line is  $S(q)$ . Generally, the behavior of  $G_0(q)$  and  $S(q)$  in the region  $q \rightarrow 0$  determines the scaling law near the percolation threshold. In principle, the free propagator behaves in the case of a massless theory as  $q^{-2}$ ; the structure factor may be a general power function  $S(q) \sim q^{-a}$ . Under this consideration there follows for the degree divergence of a vertex function  $\Gamma^{(E)}$  with  $E$  external legs

$$\Gamma \sim \kappa^{2n_4 + (2-a)l_a + (L-1)(d-6) - 2E}$$

where  $\kappa$  is a given impulse scale,  $n_4$  the number of vertices with four legs,  $l_a$  the number of structure lines, and  $L$  the number of loops. For fixed  $L$  the degree of divergence has the maximal value in the following cases:

- (a)  $2 > a$ :  $n_4 = 0, l_a = 0$ .
- (b)  $2 = a$ :  $n_4 = 0, l_a = \text{arbitrary}$ .
- (c)  $2 < a$ :  $n_4 = 0, l_a = l_a^{\text{max}}$ .

This means that if  $a < 2$ , the structure of the  $\mathbf{c}$  distribution is irrelevant, the the scaling law of the random percolation theory is always valid for the region  $a < 2$  and therefore all critical exponents have the same values as in the random percolation theory, only the nonuniversal critical point  $p_c$  will be changed. Another situation is given with  $a = 2$ . Now, a set of new relevant diagrams follows, connected by internal structure lines, which changes the typical behavior near the sol-gel transition. In this case the problem contains relevant interaction constants  $(g_0, h_0)$ , which describe the  $\Phi^3$  interaction and the  $\xi\Phi^2$  interaction. Figure 2 shows the first elements of the diagram series for these two vertices and for  $\Gamma^2(\mathbf{k})$ .

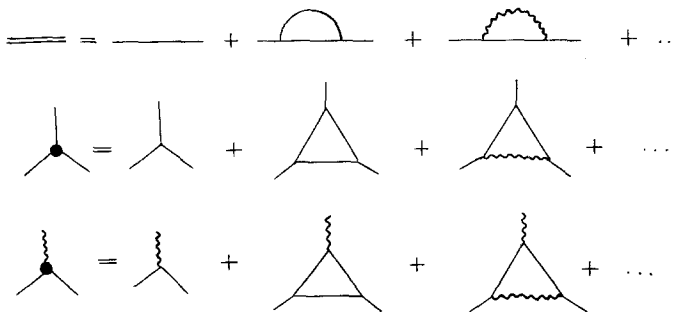


Fig. 2. Perturbation expansion for the 3 relevant vertex elements.

Using the renormalization group theory, we get the typical equation

$$\left( \kappa \frac{\partial}{\partial \kappa} + \beta_u \frac{\partial}{\partial u} + \beta_v \frac{\partial}{\partial v} - \frac{E}{2} \gamma_\phi + \gamma_{\phi^2} \mu \frac{\partial}{\partial \mu} \right) \Gamma_E = 0 \tag{10}$$

where

$$g = \kappa^{\varepsilon/2} u$$

$$h = \kappa^{\varepsilon/2} v$$

$$\mu = |p - p_c|$$

$$\varepsilon = 6 - d$$

The functions  $\beta_u$ ,  $\beta_v$ ,  $\gamma_\phi$ , and  $\gamma_{\phi^2}$  are determined by the perturbation series which are shown in Fig. 2. Using the results of the Appendix, we get the following fixpoints for the interesting case of the percolation theory  $s \rightarrow 1$ :

- (a)  $u^* = v^* = 0$ . This is the unstable Gaussian fixpoint.
- (b)  $u^* = 0$  and  $v^* \neq 0$ . Here  $(v^*)^2 < 0$ ; this fixpoint is complex and therefore an unsuitable point.
- (c)  $v^* = 0$  and  $(u^*)^2 = (2/\tau)\varepsilon + o(\varepsilon^2)$ . This is the fixpoint of the random percolation with the critical exponents  $\eta = -(1/21)\varepsilon - (206/9261)\varepsilon^2$  and  $\nu^{-1} = 2 - (5/21)\varepsilon - (653/18522)\varepsilon^2$ . This fixpoint is only stable if  $v = 0$ .
- (d)  $(u^*)^2 = \varepsilon + (13/8)\varepsilon^2$  and  $(v^*)^2 = \frac{1}{2}(u^*)^2$  is the stable fixpoint for all  $v \neq 0$ .

Hence, the last case determines the behavior near the percolation threshold for a lattice with a structure factor  $S(q) \sim q^{-2}$ . To second order, the exponents, which are calculated in a direct way, become

$$\eta = o(\varepsilon^3) \tag{11}$$

$$\nu = \frac{1}{2} + \frac{1}{8}\varepsilon + \frac{1}{32}\varepsilon^2 \tag{12}$$

Using this equations, the other critical exponents follow by the well-known scaling relations (Table I).

### 3. CONCLUSIONS

As the main result of the last considerations it follows that the behavior near the percolation transition is relatively stable against a change of the static structure factor. In the case that the structure factor is a power law  $S(q) \sim q^{-a}$  with  $a < 2$  for  $q \rightarrow 0$  (long-wave limit; small-angle

Table I. Critical Exponents

$d$	Classical	Random percolation	Percolation with $S \sim q^{-2}$
$\eta$	0	$-\frac{1}{21}\varepsilon + o(\varepsilon^2)$	$o(\varepsilon^3)$
$\nu$	$\frac{1}{2}$	$\frac{1}{2} + \frac{5}{84}\varepsilon + o(\varepsilon^2)$	$\frac{1}{2} + \frac{1}{8}\varepsilon + o(\varepsilon^2)$
$\beta$	1	$1 - \frac{1}{7}\varepsilon + o(\varepsilon^2)$	$1 + o(\varepsilon^3)$
$\gamma$	1	$1 + \frac{1}{7}\varepsilon + o(\varepsilon^2)$	$1 + \frac{1}{4}\varepsilon + o(\varepsilon^2)$
$\alpha$	-1	$-1 + \frac{1}{7}\varepsilon + o(\varepsilon^2)$	$-1 - \frac{1}{4}\varepsilon + o(\varepsilon^2)$
$\delta$	2	$2 + \frac{2}{7}\varepsilon + o(\varepsilon^2)$	$2 + \frac{1}{4}\varepsilon + o(\varepsilon^2)$
$\sigma$	$\frac{1}{2}$	$\frac{1}{2} + o(\varepsilon^2)$	$\frac{1}{2} - \frac{1}{16}\varepsilon + o(\varepsilon^2)$
$\tau$	$\frac{5}{2}$	$\frac{5}{2} - \frac{1}{14}\varepsilon + o(\varepsilon^2)$	$\frac{5}{2} - \frac{1}{16}\varepsilon + o(\varepsilon^2)$

region of X-ray scattering), one get the same unchanged critical exponents as in the case of the random percolation. Note that the scaling behavior at the percolation threshold is determined by the knowledge of  $S(q)$  for small  $q$  alone. Clearly, a change of the nonuniversal critical probability  $p_c$  will be expected. A change of the critical exponents follows for all structures with  $S(q) \sim q^{-2}$  for  $q \rightarrow 0$ . This is an important result for the formation of networks. Many amorphous systems show in the small-angle scattering region (SAXS, SANS) a typical power-like law  $S(q) \sim q^{-a}$ , which reflects the site (monomer) distribution. Hence, if this behavior is also characteristic near the sol-gel transition (determined by the bond distribution), one can expect a change of the universal behavior if  $S(q)$  scales as  $q^{-2}$ . On the other hand, if  $S(q) \sim q^{-a}$ ,  $a < 2$ , it follows the same universal class as in the random percolation theory. Because of the unknown convergence radius in the  $\varepsilon$ -expansion, further numerical simulation is desirable.

## APPENDIX

The determination of the functions  $\beta_u$ ,  $\beta_v$ ,  $\gamma_\phi$ , and  $\gamma_{\phi^2}$  follows from the calculation of the divergence part of the perturbation series in the two-loop approximation. In this case it is straightforward to calculate the connections  $g = g(g_0, h_0, \kappa)$  and  $h = h(g_0, h_0, \kappa)$  and also the field renormalization constants  $Z_\phi = Z_\phi(g_0, h_0, \kappa)$  and  $Z_{\phi^2} = Z_{\phi^2}(g_0, h_0, \kappa)$ . A simple algebraic transformation gives the dimensionless inverse relations  $u_0 = u_0(u, v)$  and  $v_0 = v_0(u, v)$  and also  $Z_\phi = Z_\phi(u, v)$  and  $Z_{\phi^2} = Z_{\phi^2}(u, v)$ . From this point and with  $g_0 = \kappa^{\varepsilon/2}u_0$  and  $h_0 = \kappa^{\varepsilon/2}v_0$ , it is simple to determine the functions

$$\beta_u = \kappa \frac{\partial u}{\partial \kappa}$$

$$\beta_v = \kappa \frac{\partial v}{\partial \kappa}$$

$$\gamma_\phi = \kappa \frac{\partial \ln Z_\phi}{\partial \kappa}$$

$$\gamma_{\phi^2} = \kappa \frac{\partial \ln Z_{\phi^2}}{\partial \kappa}$$

As a result we obtain

$$\beta_u = -\frac{\epsilon u}{2} (1 + a_1 u^2 + a_2 v^2 + a_{11} u^4 + a_{12} u^2 v^2 + a_{22} v^4)$$

$$\beta_v = -\frac{\epsilon v}{2} (1 + b_1 u^2 + b_2 v^2 + b_{11} u^4 + b_{12} u^2 v^2 + b_{22} v^4) \tag{A1}$$

$$\gamma_\phi = c_1 u^2 + c_2 v^2 + c_{11} u^4 + c_{12} u^2 v^2 + c_{22} v^4$$

$$\gamma_{\phi^2} = d_1 u^2 + d_2 v^2 + d_{11} u^4 + d_{12} u^2 v^2 + d_{22} v^4$$

with the coefficients

$$a_1 = -\frac{1}{2} z_1 + 2z_2 - \frac{7}{24} z_1 \epsilon - \frac{3}{2} z_2 \epsilon$$

$$a_2 = 5 - \frac{61}{12} \epsilon$$

$$a_{11} = z_3 - \frac{7}{8} z_1 z_2 \epsilon - \frac{49}{864} \epsilon z_1^2 - \frac{27}{8} z_2^2 - \frac{11}{12} z_1 z_2 + \frac{11}{72} z_1^2 + \frac{3}{2} z_2^2$$

$$a_{12} = -\frac{27}{8} z_1 + \frac{27}{2} z_2 - \frac{2875}{288} z_1 \epsilon - \frac{115}{8} z_2 \epsilon$$

$$a_{22} = \frac{485}{36} - \frac{8473}{432} \epsilon$$

$$b_1 = \frac{5}{3} z_1 - \frac{61}{36} z_1 \epsilon$$

$$b_2 = \frac{4}{3} - \frac{17}{9} \epsilon$$

$$b_{11} = -\frac{61}{24} z_1 z_2 \epsilon - \frac{1037}{648} z_1^2 \epsilon + \frac{8}{9} z_1 z_2 + \frac{73}{54} z_1^2$$

$$b_{12} = \frac{23}{4} z_1 - \frac{6043}{432} z_1 \epsilon$$

$$b_{22} = \frac{67}{27} - \frac{374}{81} \epsilon$$

$$c_1 = \frac{1}{6} z_1 + \frac{7}{72} z_1 \epsilon$$

$$c_2 = \frac{1}{3} + \frac{7}{36} \epsilon$$

$$c_{11} = \frac{7}{48} z_1 z_2 \epsilon + \frac{49}{2592} z_1^2 + \frac{5}{9} z_1 z_2 - \frac{11}{216} z_1^2$$

$$c_{12} = \frac{21}{8} z_1 + \frac{679}{864} z_1 \epsilon$$

$$c_{22} = \frac{109}{108} + \frac{427}{1296} \epsilon$$

$$d_1 = -z_1 + \frac{3}{4}z_1\varepsilon$$

$$d_2 = -1 + \frac{3}{4}\varepsilon$$

$$d_{11} = \frac{9}{8}z_1z_2\varepsilon + \frac{25}{32}z_1^2\varepsilon - z_1z_2 - \frac{5}{8}z_1^2$$

$$d_{12} = -\frac{11}{2}z_1 + \frac{149}{24}z_1\varepsilon$$

$$d_{22} = \frac{9}{4} + \frac{95}{48}\varepsilon$$

and

$$z_1 = s^2(s-2)$$

$$z_2 = s^3(s-3)$$

$$z_3 = s^3(s^3 - 6s^2 + 10s)$$

where  $s$  is the number of spin states ( $s=1$  for the percolation theory).

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