Correlation functions of an infinite cluster in percolation theory

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The density-density correlation function of an infinite cluster (IC) in percolation theory is calculated. The probability of finding two particles of an IC at a distance x that is small in comparison with the correlation length is of order $x^{-\zeta}$, where $\zeta = (d-2+\eta)/2$, d being the dimensionality of space ($2 \leqslant d \leqslant 6$). It is shown that the density fluctuations of an IC are described by the longitudinal spin fluctuations in the Potts model with number of states $q \to 1$, whereas the density fluctuations of clusters of finite size are described by the transverse spin fluctuations.

1 INTRODUCTION

Percolation theory is used widely for the description of polymer systems,[1] order-disorder transitions,[2] and other macroscopically disordered systems. Below the percolation-transition point in such systems there are only finite connected clusters, with a size of the order of the correlation length ξ. At the transition point ξ becomes infinite and an infinite cluster (IC) appears.

The topological structure of an IC was described in Ref. 3. The aim of the present article is to study the spatial characteristics of an IC over scales that are small in comparison with ξ and describable by correlation functions of the IC. Over larger scales the fluctuations are small; the correlation functions for this case were calculated in Ref. 4. Over distances $x \lesssim \xi$ the critical fluctuations of the particle density become strong. It is this region which is of fundamental interest in the study of the spatial characteristics of an IC. For example, the two-point correlation function $G_{\rm IC}(x) \sim x^{-\zeta}$ for $x \ll \xi$ determines important characteristics of the IC like the probability of finding two of its particles at a given distance x from each other. The higher correlation functions have an analogous meaning. In the self-consistent field approximation the critical index satisfies $\zeta = d-4$ for $d>4$ and $\zeta = 0$ for $d<4$, where d is the dimensionality of space.[4] In this article we shall show that in the fluctuation region the index ζ is not independent but is expressed in terms of other critical indices of percolation theory.

To calculate the correlation functions of an IC we shall make use of the correspondence between the percolation problem and the Potts model with q states for $q \to 1$. In the ordered phase the symmetry P_q of this model is spontaneously broken and the order parameter is nonzero. In Sec. 2 we shall show that the transverse correlation function of the order parameter coincides with the density correlation function G_F of finite (F) clusters, while the longitudinal correlation function coincides with the density correlation function $G_{\rm IC}$ of an infinite cluster. The calculation of the function $G_{\rm IC}$ performed in Sec. 3 of the article uses the self-consistent field approximation and the skeleton diagram technique in the framework of a field representation of the Potts model. In the Conclusion we discuss the region of applicability of the results obtained.

2. QUASI-AVERAGES IN PERCOLATION THEORY

We shall consider the problem of random percolation on a d-dimensional lattice. We shall denote by x the coordinates of the sites of such a lattice, and by p the probability of formation of a bond between two neighboring sites in the lattice. Such a bond is absent with probability $1-p$. The microscopic density of sites of a connected (C) percolation cluster is equal to

$$\rho_{\rm C}(\mathbf{x}) = \sum \delta(\mathbf{x}, \mathbf{x}'),$$

where δ is the Kronecker symbol and the summation is performed over the coordinates $\mathbf{x}'$ of all the sites of the connected cluster. We define the two-point correlation function by the expression

$$G(\mathbf{x}_1\mathbf{x}_2) \equiv \sum_{\rm C} \langle \rho_{\rm C}(\mathbf{x}_1)\rho_{\rm C}(\mathbf{x}_2)\rangle$$
$$= \langle \rho_{\rm IC}(\mathbf{x}_1)\rangle\langle \rho_{\rm IC}(\mathbf{x}_2)\rangle + G_{\rm IC}(\mathbf{x}_1\mathbf{x}_2) + G_F(\mathbf{x}_1\mathbf{x}_2),$$
$$G_{\rm IC}(\mathbf{x}_1\mathbf{x}_2) = \langle \Delta\rho_{\rm IC}(\mathbf{x}_1)\Delta\rho_{\rm IC}(\mathbf{x}_2)\rangle, \quad (1)$$

where the averaging is performed over all possible configurations of bonds and the function G_F is called the connectedness function of the finite clusters. To calculate the correlation function $G_{\rm IC}$ of interest, i.e., the correlation function of the density of sites of the IC, we make use of the correspondence between the percolation problem and the Potts model with q states,[5] the Hamiltonian of which in the spin formulation has the form

$$H^{(\sigma)}\{\mathbf{S}(\mathbf{x})\} = -k\sum_{\langle \mathbf{x},\mathbf{x}'\rangle} \mathbf{S}(\mathbf{x})\mathbf{S}(\mathbf{x}') - h\sum_{\mathbf{x}} \mathbf{S}(\mathbf{x})\mathbf{e}^{(\sigma)}, \quad (2)$$

where the first sum is taken over nearest neighbors and the spin $\mathbf{S}(\mathbf{x})$ at site $\mathbf{x}$ is equal to one of the q vectors $\mathbf{e}^{(\sigma)}$ directed from the center to the vertices of a $(q-1)$-dimensional tetrahedron:

$$\sum_{\sigma=1}^{q} e_\alpha^{(\sigma)} = 0, \quad \sum_{\alpha=1}^{q-1} e_\alpha^{(\sigma)} e_\alpha^{(\sigma')} = \delta(\sigma,\sigma') - q^{-1}, \quad \sum_{\sigma=1}^{q} e_\alpha^{(\sigma)} e_\beta^{(\sigma)} = \delta_{\alpha\beta}. \quad (3)$$

The percolation problem corresponds to the limit $q \to 1$ of the Potts model (2), and in this limit $p = 1 - \exp(-k/T)$, where T is the temperature.

For $h=0$ the Hamiltonian (2) is symmetric under a discrete group of rotations of the spin $\mathbf{S}$. For $p > p_c$, which corresponds to the low-temperature ($T < T_c$) phase of the spin model (2), this symmetry is spontaneously broken and the ground state is q-fold degenerate. To describe a system with degeneracy of the ground state we make use of the method of quasi-averages.[6] It can be shown that the quasi-average of the spin $\mathbf{S}$ for $q \to 1$ determines the density of sites of the IC:

$$\langle S_\alpha(\mathbf{x})\rangle^{(\sigma)} \equiv \lim_{h\to 0,\, h>0} \langle S_\alpha(\mathbf{x})\rangle_{H^{(\sigma)}} = \langle \rho_{\rm IC}(\mathbf{x})\rangle e_\alpha^{(\sigma)}. \quad (4)$$

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The two-point correlation function (1) can be expressed in terms of the spin correlator:

$$G(\mathbf{x}_1\mathbf{x}_2)=\lim_{q\to 1}\frac{\langle \mathbf{S}(\mathbf{x}_1)\mathbf{S}(\mathbf{x}_2)\rangle}{q-1}\Big|_{h=0}. \quad (5)$$

Following Ref. 7, we give for completeness a brief derivation of the relation (5). We represent the spin correlation function in the form

$$G(\mathbf{x}_1\mathbf{x}_2)=Z^{-1}\operatorname{Sp}_{\{\sigma\}}\prod_{\langle \mathbf{x},\mathbf{x}'\rangle}[1-p+p\delta(\sigma_{\mathbf{x}},\sigma_{\mathbf{x}'})]\frac{\delta(\sigma_{\mathbf{x}_1},\sigma_{\mathbf{x}_2})-q^{-1}}{q-1}, \quad (6)$$

where Z is the partition function. The expression under the trace can be represented in the form of a sum of terms, with each of which we can identify a corresponding configuration of bonds in the percolation problem. Calculating the trace in each of these configurations, we find the relation (5).

In the ordered phase the thermodynamic limit and the limit $h\to 0$ cannot be interchanged. To take account of the contribution of the IC to (5) we must set $h=0$ directly in the Hamiltonian (2). The spin correlator for $p>p_c$ and $h=0$ is equal to the sum of the quasi-averages in each of the ground states:

$$\langle S_\alpha(\mathbf{x}_1)S_\beta(\mathbf{x}_2)\rangle=\sum_{\sigma=1}^{q}\langle S_\alpha(\mathbf{x}_1)S_\beta(\mathbf{x}_2)\rangle^{(\sigma)}. \quad (7)$$

Since in the ground state of type σ the spin $\mathbf{S}$ (4) has a definite direction $\mathbf{e}^{(\sigma)}$ we must distinguish the fluctuations of its modulus and of its direction. Therefore, the spin correlation function has the form

$$\langle S_\alpha(\mathbf{x}_1)S_\beta(\mathbf{x}_2)\rangle^{(\sigma)}=\langle S_\alpha(\mathbf{x}_1)\rangle^{(\sigma)}\langle S_\beta(\mathbf{x}_2)\rangle^{(\sigma)}+G_{\mathrm{IC}}(\mathbf{x}_1\mathbf{x}_2)e_\alpha{}^{(\sigma)}e_\beta{}^{(\sigma)}+G_F(\mathbf{x}_1\mathbf{x}_2)\delta_{\alpha\beta}. \quad (8)$$

Here the functions G_{IC} and G_F describe, respectively, the longitudinal and transverse fluctuations of the spin $\mathbf{S}$. Substituting (8) and (4) into (7) and (5) and comparing with (1), we find that in the limit $q\to 1$ the functions G_{IC} and G_F in (8) are equal to the density-density correlation function of the IC and to the connectedness function of finite clusters, respectively.

3. CORRELATION FUNCTIONS OF AN INFINITE CLUSTER

To calculate the spin correlation function (8) we make use of the field representation of the Potts model.[8] For this, by means of a Hubbard–Stratonovich transformation of the term quadratic in $\mathbf{S}$ in the Hamiltonian (2), we introduce the field $\varphi_\alpha(\mathbf{x})=\langle S_\alpha(\mathbf{x})\rangle$, after which we calculate the trace over $\{\sigma\}$ in (6). The Lagrangian of the field φ_α takes the form

$$L\{\varphi_\alpha\}=\frac{\theta}{2}\sum_{\mathbf{x},\mathbf{x}',\alpha}\lambda^{-1}(\mathbf{x}-\mathbf{x}')\varphi_\alpha(\mathbf{x})\varphi_\alpha(\mathbf{x}')-\sum_{\mathbf{x}}\ln\Big[\sum_\sigma\exp\Big(\theta\sum_\alpha\varphi_\alpha(\mathbf{x})e_\alpha^{(\sigma)}\Big)\Big]. \quad (9)$$

Here $\theta=kzT$, z is the number of nearest neighbors, and the function $\lambda(\mathbf{x}-\mathbf{x}')$ is equal to $1/z$ if $\mathbf{x}$ and $\mathbf{x}'$ are nearest neighbors, and equal to zero otherwise. The spin correlation function (5) can be expressed in terms of correlators of the field φ_α.

$$\langle S_\alpha(\mathbf{x})S_\beta(\mathbf{x}')\rangle=\sum_{\mathbf{y},\mathbf{y}'}\lambda^{-1}(\mathbf{x}-\mathbf{y})\lambda^{-1}(\mathbf{x}'-\mathbf{y}')\langle\varphi_\alpha(\mathbf{y})\varphi_\beta(\mathbf{y}')\rangle-\lambda^{-1}(\mathbf{x}-\mathbf{x}'). \quad (10)$$

When fluctuations of the field φ_α are neglected the magnitude of the field is found by minimizing the Lagrangian (9). For $q=1$ we obtain

$$\langle\varphi_\alpha\rangle^{(\sigma)}=\varphi e_\alpha{}^{(\sigma)},\quad \varphi=1-\exp(-\theta\varphi). \quad (11)$$

A nontrivial solution of the equation for $\varphi=\langle\rho_{\mathrm{IC}}\rangle=1-\langle\rho_F\rangle>0$ exists only for $p>p_c=1-\exp(-1/z)$. Calculating the correlation function (8) in this self-consistent field approximation, we find for the Fourier components of the transverse and longitudinal spin correlation functions (8) the expressions

$$G_{F,\mathbf{p}}=\langle\rho_F\rangle/[1-\lambda_{\mathbf{p}}\theta\langle\rho_F\rangle],\quad \lambda_{\mathbf{p}}=\sum_{\mathbf{x}}\lambda(\mathbf{x})e^{i\mathbf{p}\mathbf{x}},$$
$$G_{\mathrm{IC},\mathbf{p}}=\langle\rho_{\mathrm{IC}}\rangle\langle\rho_F\rangle/[1-\lambda_{\mathbf{p}}\theta\langle\rho_F\rangle]^2. \quad (12)$$

The correlators (12) determine the probabilities that two points $\mathbf{x}$ and $\mathbf{x}'$ are linked together to a continuum path passing through a finite and an infinite cluster, respectively:

$$P_F(\mathbf{x}-\mathbf{x}')=G_F(\mathbf{x}-\mathbf{x}')/\langle\rho_F\rangle,\quad P_{\mathrm{IC}}(\mathbf{x}-\mathbf{x}')=G_{\mathrm{IC}}(\mathbf{x}-\mathbf{x}')/\langle\rho_{\mathrm{IC}}\rangle.$$
$$P_{\mathrm{IC}}(\mathbf{x}-\mathbf{x}')=\sum_{\mathbf{x}''}P_F(\mathbf{x}-\mathbf{x}'')\langle\rho_F(\mathbf{x}'')\rangle P_F(\mathbf{x}''-\mathbf{x}'). \quad (13)$$

Equation (13) shows that in the self-consistent field approximation an IC can be regarded as an aggregate of clusters of finite size. The local structure of an IC near each of the points $\mathbf{x}$ and $\mathbf{x}'$ is the same as that in these finite clusters, and is described by the corresponding factors P_F in (13). The summation over the common coordinate $\mathbf{x}''$ of these clusters takes account of the fact that in reality these clusters are parts of one IC.

Neglect of the fluctuations of the field φ_α is valid for $z\gg 1$, not too close to the transition point. To study the spatial characteristics of the IC in the fluctuation region we expand the Lagrangian (9) in powers of the field φ_α:

$$L\{\varphi_\alpha\}=\int\frac{d\mathbf{x}}{a^d}\Big[\frac{\tau}{2}\sum_\alpha\varphi_\alpha{}^2+\frac{a^2}{2}\sum_\alpha(\nabla\varphi_\alpha)^2-\frac{\lambda}{6}\sum_{\alpha,\beta,\gamma}d_{\alpha\beta\gamma}\varphi_\alpha\varphi_\beta\varphi_\gamma\Big],$$
$$d_{\alpha\beta\gamma}=\sum_{\sigma=1}^{q}e_\alpha^{(\sigma)}e_\beta^{(\sigma)}e_\gamma^{(\sigma)}. \quad (14)$$

Here a is the lattice constant and parameters τ and λ depend on the lattice type.

For $p<p_c$, over distances small in comparison with the correlation length $\xi\simeq a|\tau|^{-\nu}$, with $\tau\simeq p_c-p$, the correlation functions of the field φ_α have the asymptotic forms

$$\langle\varphi_\alpha(\mathbf{x}_1)\varphi_\beta(\mathbf{x}_2)\rangle=G(x_{12})\delta(\alpha,\beta), \quad (15)$$

$$\langle\varphi_\alpha(\mathbf{x}_1)\varphi_\beta(\mathbf{x}_2)\varphi_\gamma(\mathbf{x}_3)\rangle=G(\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3)d_{\alpha\beta\gamma}, \quad (16)$$

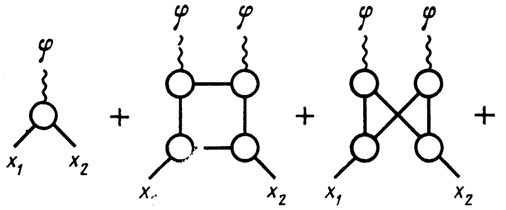
where

$$G(x_{12})=g_2x_{12}{}^{-(d-2+\eta)},\quad G(\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3)=g_3(x_{12}x_{23}x_{31})^{-(d-2+\eta)/2};$$

ν, η, and β are critical indices of percolation theory. At $p>p_c$ a condensate appears:

$$\langle \varphi_\alpha \rangle^{(\sigma)} = \varphi e_\alpha{}^{(\sigma)}, \quad \varphi = \langle \rho_{\rm IC} \rangle \sim (-\tau)^\beta,$$

and the perturbation-theory diagram technique should include condensate lines. Their contribution to the self-energy part is determined by the skeleton-diagram series in the figure. For $x_{12} \ll \xi$ the solid lines correspond to the function



(15), and the scaling asymptotic form of the vertex is

$$\Gamma_{\alpha\beta\gamma}(\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3) = \Gamma(\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3)\, d_{\alpha\beta\gamma},$$

$$\Gamma(\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3) = \prod_{i=1}^{3} \int d\mathbf{x}_i{}'\, G^{-1}(\mathbf{x}_i - \mathbf{x}_i{}')\, G(\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3), \qquad (17)$$

where the three-point correlation function is defined in (16). It is not difficult to see that for $x_{12} \ll \xi$ a contribution to the self-energy part comes only from the first diagram, which contains the smallest number of integrations over the coordinates of condensate lines. For the spin correlator we find the expression (8), where the functions G_F and $G_{\rm IC}$ for $x \ll \xi$ are equal to

$$G_F(\mathbf{x}) = g_2 x^{-(d-2+\eta)}, \quad G_{\rm IC}(\mathbf{x}) = (g_3\varphi/g_2)\, x^{-(d-2+\eta)/2}. \quad (18)$$

Thus, the correlation function G_F of the fluctuations of the direction of **S** in the ordered phase falls off more rapidly with distance than does the correlation function $G_{\rm IC}$ of the fluctuations of the amplitude S. We emphasize an important difference between this behavior of the Potts model with discrete symmetry P_q, $q \to 1$, and the behavior of the model of an isotropic ferromagnet with the continuous symmetry group $O(n)$, for which, for $x \ll \xi$, the correlation function of all the fluctuations follows the same law.[9]

According to the hypothesis of scale invariance,[10] over distances $x \simeq \xi$ the mean square fluctuation of the spin **S** is comparable to the equilibrium value of the spin:

$$G_F(\xi) \approx G_{\rm IC}(\xi) \approx \varphi^2.$$

This condition makes it possible to determine the coefficients of proportionality in (18). As a check on the scaling formulas obtained, in them we set x equal to the minimum scale a:

$$G_F(a) \approx 1, \quad G_{\rm IC}(a) \approx \varphi.$$

This result is in agreement with the fact that, according to the definition (1), we have

$$G_F(\mathbf{xx}) = \langle \rho_F \rangle = 1 - \langle \rho_{\rm IC} \rangle, \quad G_{\rm IC}(\mathbf{xx}) = \langle \rho_{\rm IC} \rangle.$$

Over distances large in comparison with the correlation length, the function $G_{\rm IC}(\mathbf{x})$ falls off exponentially; this asymptotic form was found in Ref. 4. We note that in this case too $G_{\rm IC}(\mathbf{x})$ decreases more slowly than $G_F(\mathbf{x})$. Finally, in the Fourier representation for $2 \leqslant d \leqslant 6$ we have

$$G_{\rm IC,p} \approx \begin{cases} |\tau|^{-\gamma}(1+p^2\xi^2)^{-2}, & p\xi \ll 1, \\ |\tau|^{-\gamma}(p\xi)^{-(d+2-\eta)/2}, & p\xi \gg 1. \end{cases} \qquad (19)$$

For $d = 6$ (the upper critical dimensionality for percolation theory) the IC correlation function (19) coincides with the expression obtained in (12) in the framework of the self-consistent field approximation (see also Ref. 4).

4. CONCLUSION

Thus, the idea of spontaneous symmetry breaking in percolation systems[11] makes it possible to calculate the spatial characteristics of an IC. In polymer systems such an IC corresponds to an infinite branched molecule—a gel. In polymer concentrated polymer solutions (melts) the Ginzburg number $\tau_{\rm G}$ characterizing the size of the region of strong critical fluctuations (see, e.g., Refs. 12 and 4) is small. Far from this region ($|\tau| \gg \tau_{\rm G}$) the correlation function $G_{\rm IC}$ can be calculated in the self-consistent field approximation (12) (see also Ref. 4). We have shown that in this approximation an IC looks like an aggregate of finite clusters, which are, in reality, parts of the IC. We note that essentially the same physical picture also applies in the description of the interior of a polymer globule,[13] i.e., the condensed state of a polymer chain. In the fluctuation region ($|\tau| \lesssim \tau_{\rm G}$) the density-density correlation function of an IC is determined by the expression (19).

In systems that are far from incompressible, the density fluctuations grow as the point of gel formation is approached. A field theory describing the general case of compressible polymer systems was constructed in Ref. 4. When the density fluctuations are taken into account other vertices besides τ and λ appear in the Lagrangian (14), and grow rapidly under the action of renormalization-group transformations. These vertices can also be reproduced in the framework of the field formulation of the three-parameter Potts model,[14] the Hamiltonian of which is given by (2) with the additional term

$$-J \sum_{\langle \mathbf{x},\mathbf{x}' \rangle} (\mathbf{S}(\mathbf{x})\mathbf{e}^{(\sigma)})\,(\mathbf{S}(\mathbf{x}')\mathbf{e}^{(\sigma)}). \qquad (20)$$

As shown in Ref. 14, this model describes the statistics of finite percolation clusters—lattice animals. Thus, the density fluctuations take the polymer system out of the percolation regime and into the fluctuation regime of lattice animals.

We emphasize an important difference between this regime in polymer systems and the case of the Potts model (20). Whereas in the Potts model it describes only large finite clusters, while the connectedness function and statistical density fluctuations of the IC are controlled by the percolation regime, allowance for density fluctuations leads to the result that the lattice-animal regime also describes the properties of the infinite network of a gel.

In the self-consistent field approximation the correlation function of a swollen gel was calculated in Ref. 11. It is clear that this function will also have the same form in dilute systems in the fluctuation regime of lattice animals over scales that are large in comparison with the correlation length ξ of the system. Thus, in polymer systems percolation behavior can be observed only in a limited range of their parameters.

An experimental study of the spatial characteristics of an IC would be of great interest. In particular, the intensity of light scattering and of Bragg scattering of neutrons by an IC structure gives direct information about the correlation function (19). A two-dimensional IC can be formed, e.g., as a result of random breaking of bonds of a wire network. The properties of a three-dimensional IC can be studied by immersing into a liquid a porous material that was above the percolation threshold. In the bulk of the sample the liquid fills only the IC structure, and this makes it possible to distinguish the IC among the clusters of finite size. In polymer systems this end is achieved by washing the finite molecules out of the gel network.

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