Equation for cluster distribution in percolation theory

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An equation is deduced for the size distribution function of clusters close to the percolation threshold in the problem of "spheres." It is shown that the solution contains only one arbitrary geometric constant, which is a function of the dimensionality of the space. Asymptotic forms are found. In two models in which the distribution function is calculated, it satisfies equations similar to the one developed in this work.

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One of the most fundamental characteristics in percolation theory is the size distribution function of clusters. Such important values as the probability for a particle to belong to an infinite cluster and the mean size of finite clusters are expressed through this function. It can also define other physical characteristics (see Ref. 1). Heretofore, all attempts to determine this function reduced to direct numerical calculation using models that as a rule presented point problems on two-dimensional lattices. There were also certain general theorems, which concerned asymptotic behavior

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far from the percolation threshold (see Ref. 2, where a list of the relevant literature is given).

This work describes the derivation of an equation for the distribution function in the vicinity of the percolation threshold, and some of its consequences. The "sphere problem" is used as a model in two or three dimensions. We formulate it as follows. Let points with density n_m be randomly scattered in space. Let us encircle each of them by a sphere with radius r_0. If these spheres intersect for two points, we will assign them to one cluster. Let us introduce the parameter $p = (4\pi/3)n_m r_0^3$. As is shown in Ref. 3, for a critical value of $p_c = 0.38 \pm 0.1$ for $d = 3$ (in Ref. 3, the value $\beta = 8p$ is actually used), an infinite cluster is formed. This is the percolation threshold. We indicate $\epsilon = (p_c - p)/p_c$. The number of clusters which contains n particles is proportional to the complete number of particles in the system (i.e., $N = n_m V$). Having divided by N, we obtain $a(n)$, which we shall call cluster distribution function.

Near the percolation threshold ($|\epsilon|T \ll 1$) and for large clusters ($n \gg 1$), the distribution function should have a self-similar form[4] (see also Ref. 1)

$$a(n) = \frac{1}{n^b} f(\epsilon n^a), \tag{1}$$

where the function $f(x)$ is analytical for $x \to 0$, and decreases for $x \to \pm\infty$. Reference 1 presents the conditions for normalizing the function f and its relationship with the basic parameters of percolation theory.

The equation for $a(n)$ can be obtained from the following considerations. Let us increase slightly the interaction radius r_0. In so doing, we cause the merging of some clusters. The number of clusters with n-particles will increase due to the merging of smaller clusters, and it will decrease due to the adhesion of n-clusters to other finite clusters, or to an infinite cluster (for $\epsilon < 0$). If the process of merging could occur with any particles of each cluster, the probability of the process would be proportional to the product of the probabilities of particles belonging to the corresponding clusters. Such a probability equals $na(n)$ ($Na(n)$ clusters with n-particles, $nNa(n)$ particles in n-cluster). Actually, however, the particles of the inner parts of the cluster or of the surfaces of deep "fjords" are ineffective, and therefore the probability of merging of clusters with n_1- and n_2-particles can be set proportional to $n_1^q a(n_1) \times n_2^q a(n_2)$ where, for the d-dimensions $(d-1)/d < q < 1$.

The foregoing leads to the following equation:

$$-\frac{\partial a(n)}{\partial \epsilon} = \frac{1}{2}\sum_{m=1}^{n-1} m^q a(m)(n-m)^q a(n-m) - n^q a(n)\left[\sum_{m=1}^{\infty} m^q a(m) + S(\epsilon)\right], \tag{2}$$

where $S(\epsilon)$ is the probability of the particle belonging to the effective part of an infinite cluster. The constant coefficient in the probability of merging is included in ϵ.

When $\epsilon > 0$, $S(\epsilon) = 0$. Multiplying Eq. (2) by n and performing a summation from 1 to ∞, we obtain $(\partial/\partial\epsilon)\Sigma_{n=1}^{\infty} na(n) = 0$, which corresponds to the normalization condition. Regrouping the terms, we obtain

$$-\frac{\partial a(n)}{\partial \epsilon} = \sum_{m=1}^{n/2} m^q a(m) [(n-m)^q a(n-m) - n^q a(n)]$$

$$- n^q a(n) [\sum_{n/2}^{\infty} m^q a(m) + S(\epsilon)]. \qquad (3)$$

In this form, it is clear that when $n \gg 1$, only $m \gg 1$ exist in the summation, which makes it possible to turn to integrals.

Because the merging of the clusters has no effect on the total number of effective particles, the following relationship holds

$$\sum_{n=1}^{\infty} n^q [a(n,\epsilon) - a(n,0)] = -S(\epsilon). \qquad (4)$$

This makes it possible to write Eq. (3) in another form

$$-\frac{\partial a(n,\epsilon)}{\partial \epsilon} = \int_0^{n/2} m^q a(m,\epsilon) [(n-m)^q a(n-m,\epsilon)$$

$$- n^q a(n,\epsilon)] dm + n^q a(n,\epsilon) \xi \int_0^{n/2} m^q [a(m,\epsilon) - a(m,0)] dm \qquad (5)$$

$$- \int_{n/2}^{\infty} m^q a(m,0)\, dm.$$

Finally, using

$$\sum_{n=1}^{\infty} n [a(n,\epsilon) - a(n,0)] = -P(\epsilon), \qquad (6)$$

where $P(\epsilon)$ is the probability of a particle belonging to an infinite cluster (see Ref. 1) for $\epsilon < 0$, we obtain from Eq. (3)

$$\frac{\partial P}{\partial |\epsilon|} = S(|\epsilon|) \sum_{n=1}^{\infty} n^{q+1} a(n). \qquad (7)$$

From the theory of similarity, it follows that

$$P(\epsilon) = p|\epsilon|^{\beta} \theta(-\epsilon), \quad S(\epsilon) = s|\epsilon|^{\delta} \theta(-\epsilon). \qquad (8)$$

Substitution of $\alpha(n)$ as it appears in Eq. (1) into Eqs. (3) or (5), as well as Eqs. (4), (6) and (7) yields the following:

a) equations

$$-\frac{\partial f}{\partial x} = \int_0^{1/2} u^{-\xi} f(xu^a) \{(1-u)^{-\xi} f[x(1-u)^a] - f(x)\} du$$

$$- fx \int_{1/2}^{\infty} u^{-\xi} f(xu^a) du - f(x)\,\theta(-x)\, s\, x^{\delta} \qquad (3')$$

$$-\frac{\partial f}{\partial x} = \int_0^{1/2} u^{-\xi} f(xu^a) \{(1-u)^{-\xi} f[x(1-u)^a] - f(x)\} du$$

$$+ f(x) \int_0^{1/2} u^{-\xi} [f(xu^a) - f(0)] du - f(x) f(0) \int_{1/2}^{\infty} u^{-\xi} du, \qquad (5')$$

b) relationships between the exponents where $\xi = b - q$,

$$a = 2q + 1 - b, \quad \delta = \frac{q}{a} - 1, \quad \beta = \frac{b-2}{a}, \qquad (8)$$

c) additional conditions applicable to the solution

$$\int_0^{\infty} x^{1-\frac{q}{a}} f'(x) dx = 0$$

$$\frac{1}{q-a} \int_0^{\infty} x^{1-\frac{q}{a}} f_1'(x) dx = \int x^{1-\frac{2q-1}{a}} f_1'(x) dx \Big/ \left[\int_0^{\infty} x^{\frac{1-q}{a}} f_1(x) dx\right], \qquad (9)$$

where $f_1(x) = f(-x)$, and

d) expressions for the constants p and s through $f_1(x)$, which we will not introduce.

Substituting in Eq. (5′)

$$f(x) = \sum_{s=0}^{\infty} f_s x^s, \qquad (10)$$

we obtain a family of equations

$$-(s+1) f_{s+1} = \left(\frac{1}{2}\right)^{1+as-2\xi} \sum_{s_1=0}^{s} f_{s_1} f_{s-s_1} \cdot$$

$$\left[\frac{1}{1+s_1 a - \xi} + \frac{a(s-s_1)-\xi}{1+as_1-\xi} \int_0^1 u^{s_1 a+1-\xi} (2-u)^{a(s-s_1)-1-\xi} du\right]. \qquad (11)$$

Thus, all f_s are expressed thru f_0. Consequently, the following unknowns remain: q, f_0, and α. The index q is a function of the number of dimensions. Numerical calculations yield $q = 0.83 \pm 0.03$ ($d = 3$) and $q = 0.73 \pm 0.01$ ($d = 2$). For a given value of q, conditions (9) determine both f_0 and α.

The asymptotic forms of $f(x)$ for $x \to \pm \infty$ are obtained from Eq. (3'):

1) $f(x) \approx c\, x^{\nu} \exp(-t\, x^{1/a}), \quad x \to \infty$

$$\nu = \frac{1}{a} - 1, \quad \frac{t}{a} = c\,\phi(q), \quad \phi(q) = \int_0^{1/2} u^{-q} (1-u)^{-q}\, du$$

2) $$f(x) \approx c_1 x^{\nu_1} \exp(-t_1 |x|^{q/a}), \quad x \to -\infty \quad t_1 = \frac{q}{a} s \qquad (12)$$

These formulas are consistent with the general forms and to results of the numerical calculations (see Ref. 2). There are two models which permit immediate calculation of the function $\alpha(n)$: the Bethe lattice ($b = 5/2$, $\alpha = \frac{1}{2}$, $f(x) = \exp(-x^2/2)$[5] and the one-dimensional problem of "spheres" ($a(n) = \lambda^2 (1-\lambda)^{n-1}$, $\lambda = \exp(-n_m \Delta)$, ($\Delta$ is the radius of interaction) (see Ref. 6). In the first case, $f(x)$ satisfies Eq. (3') with $q = 1$ (supplementary conditions (9) do not pertain to this case). In the second case, $\alpha(n)$ satisfies Eq. (3) with the left-hand side $-(\lambda^2/2)(\partial\alpha(n)/\partial\lambda)\, q = 0$, $S_{(\epsilon)} = 0$, $\lambda = 0$ corresponds to the percolation threshold; the area below the threshold is nonexistent. The fact that the proposed approach is confirmed in two limiting cases ($q = 0$ and $q = 1$) is convincing proof of its correctness.

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