The relation between the critical exponents of percolation theory

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A scaling hypothesis in percolation theory is formulated, making it possible to relate the correlation-length index to the exponents of the infinite-cluster density and of the mean finite-cluster size. To check the relation obtained the correlation-length index is calculated for the site problem in the two-dimensional and three-dimensional cases on a computer by the Monte Carlo method. The results of the calculation confirm the scaling hypothesis.

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1. In recent years the ideas and results of percolation theory have found wide use in the physics of disordered systems[1-4]. One of the simplest problems of percolation theory—the site problem—is formulated as follows. We consider an infinite periodic lattice, over the sites of which zeros and ones are distributed in a random manner. Let the fraction of sites occupied by ones be x. Two ones are regarded as connected if they are nearest neighbors. We say that all ones connected together both directly and through chains of other pairwise-connected ones belong to one cluster. We require to find the critical value x_c of the concentration x of ones at which an infinite cluster of ones is first formed, or, in other words, at which percolation with respect to the ones arises.

The position of the percolation threshold x_c has been well studied for different lattices. It has also been established that, immediately beyond the threshold, i.e., for $0 < x - x_c \ll 1$, the fraction P(x) of lattice sites belonging to an infinite cluster increases according to the power law:

$$P(x) \sim (x-x_c)^{\beta}, \tag{1}$$

in which, according to[4, 5], β depends on the dimensionality d of space:

$$\beta=0.35\pm0.05 \text{ for } d=3, \tag{2a}$$

$$\beta=0.14\pm0.03 \text{ for } d=2. \tag{2b}$$

The result (2a) is the same for three different lattices.

The problem under consideration is analogous to a second-order phase transition. If we use the language of ferromagnetic transitions, P(x) obviously corresponds to the spontaneous magnetization and x_c to the transition temperature. The region $x < x_c$ corresponds to the paramagnetic region, and the region $x > x_c$ to the ferromagnetic region.

The analogy with a phase transition has been elucidated more fully by Kasteleyn and Fortuin[6]. They introduced the parameter h, playing the role of the dimensionless magnetic field $\mu H/T$, where μ is the spin magnetic moment. We imagine an extra site occupied by a one (the demon of Kasteleyn and Fortuin), which does not belong to the lattice under consideration but, by definition, is connected with each of its ones with probability $1-e^{-h}$. It is clear that in the presence of the demon an infinite cluster exists for arbitrarily small x. For $x \to 0$ and $h \ll 1$ the function $P(x, h) \to xh$. The number of finite clusters per lattice site can be written in the form

$$F(x, h)=\sum_s n_s e^{-hs}, \tag{3}$$

where n_s is the number (per lattice site) of finite clusters with s ones for h = 0. The factor e^{-hs} is the fraction of clusters of size s in which not one of the sites is connected with the demon.

The quantity F(x, h) is analogous to the free energy of the ferromagnet. Indeed, the order parameter P(x) is determined by the derivative $\partial F/\partial h$ at h = 0:

$$P(x)=x-\sum_s sn_s=x+\left.\frac{\partial F}{\partial h}\right|_{h=0}. \tag{4}$$

We introduce the mean size of the finite cluster to which an arbitrarily chosen unity belongs:

$$S(x)=\sum_s s^2 n_s. \tag{5}$$

According to (3),

$$S(x)=\left.\frac{\partial^2 F}{\partial h^2}\right|_{h=0}. \tag{6}$$

It follows from (6) that the quantity S(x) is analogous to the susceptibility. Its behavior in the pre-threshold region has been well studied. According to[7], for $x \to x_c - 0$,

$$S(x) \sim (x-x_c)^{-\gamma}, \tag{7}$$

where, for all the lattices investigated

$$\gamma=1.69\pm0.03 \text{ for } d=3, \quad \gamma=2.38\pm0.05 \text{ for } d=2. \tag{8}$$

Differentiating F(x, h) with respect to both variables, we can obtain a set of functions analogous to all the remaining thermodynamic quantities studied in the theory of critical phenomena.

Up to now we have discussed the site problem. The other problems of percolation theory differ from this in the character of the arrangement of the sites and of the ones, and in the rules establishing the linking of the ones with each other[1]. In these problems quantities analogous to x, P(x), S(x) and F(x, h) can be introduced. The fact that the indices β and γ are independent of the lattice type prompts the thought[7] that the indices of percolation theory are universal for all problems and are determined only by the dimensionality of space. This assumption corresponds to the hypothesis of universality in the theory of phase transitions, which postulates that the character of the interaction at short distances has a weak effect on the critical indices. It is true that, in the theory of phase transitions, for a given dimensionality of space there remains a weak dependence of the indices on the number of components of the order parameter; e.g., the difference between the Ising and Heisenberg problems is connected with this. On the other hand, all the problems known to us in percolation theory are one-component problems, so that the corresponding discrepancies between the indices should be absent. The existing data do not contradict the hypothesis of universality.

Essam and Gwilym[8] have formulated a scaling hypothesis for the quantity F(x, h). They postulated that

$$F=\tau^a\Phi(\tau/h^b), \tag{9}$$

where $\tau = (x - x_c)/x_c$. This assumption is sufficient to relate the indices of the derivatives of $F(\tau, h)$ with respect to τ and h. However, up to now, only two such indices (β and γ) have been studied, and this is insufficient to check the scaling hypothesis. On the other hand, in percolation theory there exists another quantity–the correlation length. This quantity becomes infinite at the threshold point ($L \sim \tau^{-\nu}$).

It has been shown [9,10] that the pre-exponential factor in the hopping conductivity and the exponent in the expression for the electrical conductivity of a thin film are expressed in terms of the correlation-length index ν. In[11] the correlation length was introduced by treating percolation in finite volumes. (In an analogous way, in the theory of phase transitions the correlation length is studied from the smearing-out of the specific-heat singularity near the transition point in finite volume[12].) This is a constructive method which makes it possible to determine the index ν by means of computer calculations by the Monte Carlo method. Using a calculation of Kurkijärvi[13], the authors of[11] found that for d = 3 the index $\nu = 0.83 \pm 0.13$.

In this paper we shall introduce a correlation function into percolation theory, thereby giving a definition of the correlation length in the traditional form. We then extend the scaling hypothesis in such a way that the transformation law for the correlation function follows from it. In this form the formulation of the scaling hypothesis turns out to be analogous to that of Kadanoff[14]. The new formulation makes it possible to relate the index ν to the indices β and γ. As a result it becomes possible to check the scaling hypothesis. In the three-dimensional case we can use for this purpose the above-mentioned calculation of[13]. However, its accuracy is not great. In addition, it would be desirable to check the hypothesis of universality with respect to the different problems of percolation theory. In the two-dimensional case the index ν has not been calculated. For these reasons we have undertaken calculations of the index ν of the site problem for the simple-cubic and square lattices on a computer by the Monte Carlo method. The result of this check confirms the scaling hypothesis.

2. We shall define the quantity $g(\mathbf{r}, \mathbf{r}')$ on the lattice sites, putting it equal to unity if the sites $\mathbf{r}$ and $\mathbf{r}'$ are occupied by ones and belong to the same finite cluster, and equal to zero in all other cases. After this we introduce the correlation function $G(\mathbf{r} - \mathbf{r}', x)$ by averaging $g(\mathbf{r}, \mathbf{r}')$ over all the lattice sites:

$$G(\mathbf{r}-\mathbf{r}', x)=\langle g(\mathbf{r}, \mathbf{r}')\rangle. \tag{10}$$

Obviously, $G(\mathbf{r}, x) \to 0$ as $r \to \infty$. We shall assume that it contains a single characteristic length, which we shall call the correlation length L. The divergence of the correlation length as $x \to x_c$ characterizes the increase of the mean size of the clusters as the percolation threshold is approached. For $x > x_c$ the correlation length also describes the characteristic size of the mesh which is formed by the infinite cluster. From the definitions (10) and (5) follows the important relation

$$S(x)=\sum_{\mathbf{r}} G(\mathbf{r}, x), \tag{11}$$

which is completely analogous to the well-known relation for the susceptibility[14].

We turn now to the formulation of the scaling hypothesis. By analogy with the theory of phase transitions[14] we shall assume that the singular parts of the functions F and G satisfy the relations

$$F(\tau l^y, hl^z)=l^d F(\tau, h), \tag{12}$$

$$G(r, \tau)=l^{-d+2-\eta}G(rl^{-1}, \tau l^y), \tag{13}$$

where y, z and η are as-yet unknown indices. From (12) follows (9), with a = d/y and b = y/z. By means of (12), (13), (4), (6) and (11), all the indices of percolation theory can be expressed in terms of two indices, e.g., y and z. We shall not write out all the relations between the indices, which are completely analogous to the relations following from the static scaling hypothesis[14]. For us, only the relation connecting the three indices investigated is important now:

$$d\nu=\gamma+2\beta. \tag{14}$$

3. To determine the index ν we have studied percolation in finite volumes for the two- and three-dimensional cases. For finite volumes the percolation threshold x_c varies from realization to realization. Let l be the number of sites along a side of the square of cube in which the percolation is being studied. The dispersion of the percolation threshold is determined by the formula $W_l^2 = \langle (x_c - \langle x_c \rangle)^2 \rangle$, where $\langle .. \rangle$ denotes averaging over the different realizations for a given value of l. As $l \to \infty$, W_l decreases with increasing l in accordance with the law[11]

$$W_l=B/l^{1/\nu}, \tag{15}$$

where B is a constant and the index ν coincides with the correlation-length index. Thus, the index ν can be determined by studying the dispersion of the percolation in large volumes.

We have calculated W_l analytically for $l = 1$ and $l = 2$ only. For larger values of l numerical calculations were carried out on a BÉSM-6 computer by the Monte Carlo method. Numerical calculations were also performed for $l = 2$ for the purpose of checking the program. Their results coincided with the results of the analytical calculation.

We used a program compiled in accordance with the algorithm described earlier[15]. Calculations were performed for the simple-square and simple-cubic lattices.

For the two-dimensional case the percolation was studied in squares with sides equal to 4, 8, 16, 32, 64, 128 and 256. The results of the calculations are given in Table I. In Fig. 1 we give the distribution functions (normalized in the same way) for the threshold value x_c for $l = 8$, 32 and 128. The calculated third and fourth moments of the distribution functions for $l = 16$, 32, 64 and 128 coincide to within the fourth decimal place with the corresponding moments of the Gaussian distribution function. Approximately 0.68 of the total number of realizations fall in the interval $2W_l$ centered at the maximum of the distribution, and approximately 0.95 of the total

TABLE I. Results of percolation calculations for the two-dimensional case

l	Number of realizations n	Mean value $\langle x_c \rangle$	Dispersion W_l
1	Analytic calculation	$^1/_2$	0.289
2	Analytic calculation	$^8/_{15}$	0.2218
4	4000	0.565±0.003	0.155±0.002
8	1000	0.581±0.003	0.103±0.003
16	5000	0.5884±0.0002	0.0634±0.0006
32	1000	0.5924±0.0013	0.0399±0.0009
64	1000	0.5934±0.0008	0.0243±0.0005
128	180	0.593±0.001	0.0142±0.0007
256	8	0.594±0.003	–

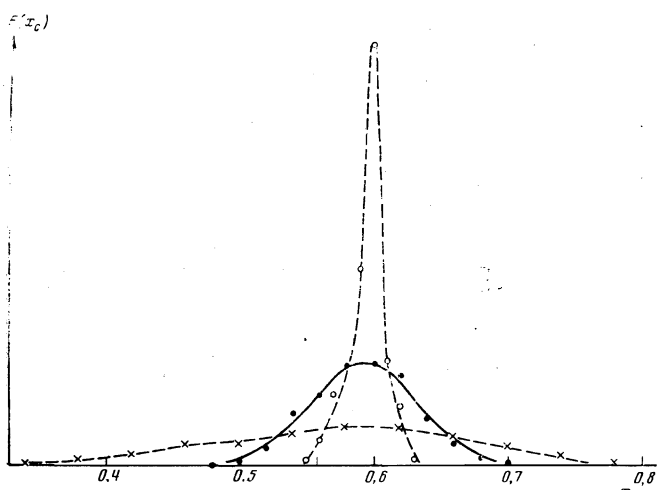

FIG. 1. Distribution function $f(x_c)$ of the percolation threshold x_c for different l: × 8; ● 32; ○ 128.

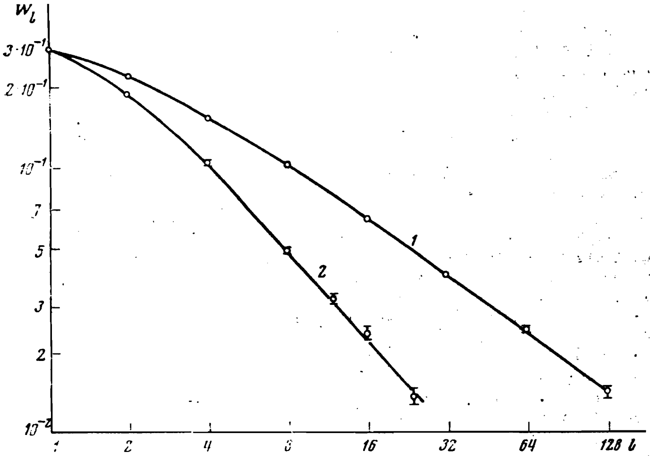

FIG. 2. Dependence of W_l on l on a doubly logarithmic scale. Curve 1—the two-dimensional case; curve 2—the three-dimensional case.

number of realizations fall in the interval $4W_l$; this coincides, within the calculational accuracy, with the corresponding values for the Gaussian distribution.

Figure 2 shows the dependences of W_l on l on a doubly-logarithmic scale for the two-dimensional (curve 1) and three-dimensional (curve 2) cases. It can be seen from the figure that as l increases these dependences asymptotically approach a straight line. The slope of the asymptote determines the quantity ν^{-1}. In the two-dimensional case, to determine this quantity with the greatest possible accuracy and to determine the magnitude of the error we have approximated the dependence shown in curve 1 of Fig. 2 by the expression $W_l = B(l + c)^{-1/\nu}$, where B = 0.54, c = 1.4 and

$$\nu=1.33\pm0.04,\quad d=2. \tag{16}$$

This is our result in the two-dimensional case.

In the three-dimensional case we have studied the percolation in cubes with sides l = 4, 8, 12, 16 and 24. The results of the calculations are presented in Table II. From Fig. 2 (curve 2) it can be seen that for $l \geq 4$ the dependence of W_l on l for the three-dimensional case is a straight line, the slope of which determines ν:

$$\nu=0.9\pm0.05,\quad d=3. \tag{17}$$

The errors ΔW_l indicated in Table II are connected with the fact that for each value of l a finite number n of realizations has been used. They were calculated from the formula

$$2W_l\Delta W_l=n^{-1/2}[\langle(x-\langle x\rangle)^4\rangle-\langle(x-\langle x\rangle)^2\rangle^2]^{1/2}. \tag{18}$$

It should be noted that the results of this calculation agreed well in all cases with the estimate $\Delta W_l = W_l/(2n)^{1/2}$,

TABLE II. Results of percolation calculations for the three-dimensional case

l	n	$\langle x_c \rangle$	W_l
1	Analytic calculation	0.5	0.289
2	Analytic calculation	0.407	0.186
4	1600	0.352±0.003	0.103±0.002
8	1000	0.335±0.002	0.0488±0.011
12	200	0.331±0.003	0.0319±0.016
14	120	0.329±0.002	0.0268±0.0017
16	170	0.320±0.002	0.0236±0.0013
24	100	0.318±0.0015	0.0136±0.0010

valid for the Gaussian distribution.

The errors in the formulas (16) and (17) were found by means of graphs of the dependences of log W_l on log$(l + c)$ for d = 2 and of log W_l on log l for d = 3. These errors are determined by the scatter of the angles of slope of the straight lines that can be drawn through the calculated points taking the errors ΔW_l into account.

4. The result (17) for d = 3 coincides with the quantity $\nu = 0.83 \pm 0.13$, mentioned in Sec. 2, for the random-site problem. This corroborates once more the universality hypothesis.

We return now to the relation (14), which follows from the scaling hypothesis. Substituting the indices β and γ from (2) and (8) into it, we obtain

$$\begin{aligned}\nu&=0.80\pm0.05 \text{ for } d=3,\\ \nu&=1.33\pm0.05 \text{ for } d=2,\end{aligned} \tag{19}$$

which agree with (16) and (17) within the error bars. Thus, within the framework of the calculations carried out so far, the scaling hypothesis is confirmed.

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