

SYSTEM OF DIFFERENTIAL EQUATIONS FOR THE LATTICE PROBLEMS OF THE PERCOLATION THEORY

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A model of cluster formation in the percolation system is proposed. On its basis a system of differential equations for finite clusters and a differential equation for an infinite cluster are obtained. The solutions of these equations for several limiting cases are investigated. A method of approximate closure of the equation for an infinite cluster using a system of equations for a number of finite clusters is developed, and an expression for the percolation probability in the entire range of change of the part of the conducting bonds in the system is obtained by means of this method.

Percolation theory as an independent branch of science arose at the end of the 1950s from the problem of percolation of a fluid through a porous medium [1]. Currently this theory enables one to solve a very wide class of problems related to different branches of science. One of the main merits of the theory is that it adequately describes many systems in which a geometrical phase transition occurs: the conductor-insulator transition in mixtures of conducting and insulating particles [2], splitting of rocks in formation of a sufficient number of cracks [3], and so on. This theory is also used in describing the elasticity of polymeric gels [4], jump conduction in alloyed semiconductors [5], Anderson localization in disordered systems [6], critical condensation in Coulomb systems [7], and in calculation of the properties of porous electrodes [8]. Every year more and more classes of problems are revealed for solution of which percolation models are used.

At the present time, a number of methods are being applied to the solution of problems of percolation theory. Most of the results in this area have been obtained by means of the Monte Carlo method. Among the analytical methods, we should note the series method of Domb and Sykes [9, 10], the method of generating functions [11], and the formalism of a renormgroup [12]. In the vicinity of the percolation threshold, the theory of scaling invariance has been successfully used [13, 14]. In percolation theory, use is also made of graph theory [8], general methods of probability theory [15], and the mean-field approximation [16]. Nevertheless, the state of the art of the theory is such that it enables one to find exact analytical solutions of percolation problems only in the simplest limiting cases (for example, in lattice problems such a solution has been found for the Bethe lattices [16], while in case of continuum problems it has been obtained for a one-dimensional model [17]). Not in the least dismissing the merits of all the methods enumerated, we suggest an alternative approach, different from the above-mentioned, ones to the solution of percolation problems. In the present work, the problem is considered in the context of the kinetic theory (a formal analogy is borne in mind). This enables one to improve part of the known results and to obtain new results for a number of cases. Some preliminary results on this subject were partially presented in [18].

1. Basic Definitions. The present work deals with the bond-percolation problem [16]. All the following derivations and conclusions can be considered to be rather general owing to the fact that they enable one to carry out a generalization to the case of the site-percolation problem.

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Let links of two types be distributed randomly in an infinite lattice of arbitrary dimensions. To be specific, we will discuss permeable and impermeable pores in a capillary lattice. It follows from the assumption of random distribution that an arbitrary pore in the lattice is permeable with probability q and impermeable with probability $(1 - q)$. Here q and $(1 - q)$ are the parts of the permeable and impermeable pores in the lattice, respectively.

Permeable pores form clusters in the lattice. Two such pores belong to the same cluster if they are interconnected by a chain of permeable pores. By an (i, j) -cluster is meant a connected system of i conducting pores bounded by j nonconducting pores on all sides. The numbers i and j are called the cluster size and the perimeter. In addition to clusters of finite size, a cluster of infinite size, i.e., an infinite connected system of permeable pores or a simply infinite cluster (IC) can exist in the lattice.

Let n'_{ij} be the number of the (i, j) -clusters in the lattice of N bonds (the primed quantity implies the absolute number of clusters of a particular kind in the system and the unprimed one denotes that the quantity has already been normalized to the number of bonds or the number of sites in the system). Then the probability Q_{ij} of an arbitrary bond belonging to the (i, j) -cluster is equal to

$$Q_{ij} = \frac{in'_{ij}}{N} = in_{ij}. \quad (1)$$

Let n'_k be the total number of clusters containing k sites. The following relation can be written for n_k :

$$n_k = \frac{z}{2} \sum_{\{2i+j=kz\}} n_{ij} = \frac{z}{2} \sum_{\{2i+j=kz\}} \frac{a_{ij}}{i} q^i (1 - q)^j. \quad (2)$$

Here the well-known expression for n_{ij} [16] is used (the meaning of the coefficients a_{ij} is also clarified in the work mentioned), n_k is normalized to the total number of sites in the lattice, and the condition of summation is written in curly brackets under the summation sign. Then the probability of an arbitrary site belonging to the cluster containing k sites (the k -cluster) is equal to

$$Q_k = \frac{kn'_k}{2N} z = kn_k, \quad (3)$$

(since the lattice of N elements contains $2N/z$ sites).

Basic "macroscopic" characteristics of the percolation system, whose determination is one of the problems of this work, are written in the following way [16]:

$$Q_b(q) = q - \sum_{\{i,j\}} Q_{ij} = q - \sum_{\{i,j\}} \frac{in'_{ij}}{N} = q - F(q), \quad (4)$$

$$Q_p(q) = 1 - (1 - q)^z - \sum_{\{k\}} kn_k(q) = 1 - (1 - q)^z - F(q) - \frac{1}{2} S_f(q), \quad (5)$$

$$S_f(q) = \sum_{\{i,j\}} \frac{jn'_{ij}}{N}, \quad (6)$$

$$S(q) = \left(\sum_{|k|} k^2 n_k(q) \right) / \left(\sum_{|k|} k n_k(q) \right). \quad (7)$$

2. Probability of Transition of a Nonconducting Bond to a Conducting Bond with Infinitesimal Increase in the Part of the Conducting Bonds in the System. First of all, it is necessary to consider the behavior of a in individual bond with infinitesimal changes in the system. In this case, by a percolation system we mean a lattice of bonds, part of which is occupied.

Classical problems of percolation theory, which include the problems of bonds and sites, are steady-state. For the problem of bonds this means that we have the lattice with a *fixed in space* random distribution of conducting and nonconducting bonds with a given q . Because of this, it is necessary to explain precisely what is meant by the transition of a bond from one state to another.

We consider an ensemble of the percolation systems that includes a set of systems (lattices) with all possible values of a part of the conducting bonds from 0 to 1. A change in q and the related change in the properties of the system are described by means of transition from the subensemble of the systems where the part of the conducting bonds is equal to q to a subensemble with this part larger by the infinitesimal quantity dq . In our case, the transition of any bond from a nonconducting state to a conducting state means that at the site occupied by a given bond in the lattice we find a larger number of conducting bonds for the second subensemble than in the first one. It should also be noted that all the values related to both the finite clusters and the infinite one are considered as mean with respect to the corresponding subensemble.

Having analyzed several characteristic applications of the percolation theory, we arrived at the conclusion that the increase in the part of the conducting bonds (elements) q results in the transformation of some clusters to others, which obeys the following rule with a large degree of accuracy: *with increase in the part of the conducting bonds in the system, the cluster cannot break up into smaller ones (the conducting bond cannot become nonconducting)*. A consequence of this rule is that with increase in the part of the conducting bonds, clusters of larger sizes can be formed only of clusters of smaller sizes by joining of the latter.

Using this rule, we obtain the probability of transition of an arbitrary nonconducting bond to a conducting bond with infinitesimal increase in the part of the conducting bonds in the system.

Let a certain arbitrary bond of the lattice be nonconducting with a given q (the event \bar{A} , where the over bar means a contrary event, i.e., A is an event consisting of the fact that the bond selected is conducting under these conditions). We increase the part of the conducting bonds by the small quantity dq . Let \bar{B} be an event which implies that the given bond is nonconducting for the part of the conducting bonds equal to $q + dq$. The onset of the event B is of interest to us on condition that the event \bar{A} has occurred.

We write the following relations, which will be necessary in the calculations:

$$P(\bar{A}) = 1 - q, \quad P(\bar{B}) = 1 - (q + dq), \quad (8)$$

$$P(B/\bar{A}) = \frac{P(B \cap \bar{A})}{P(\bar{A})}, \quad (9)$$

$$P(\bar{A}) = P(\bar{A} \cap \bar{B}) + P(\bar{A} \cap B). \quad (10)$$

Using the above rule, we can write that $\{\bar{B} \setminus \bar{A}\} = \{0\}$ (here $\{\bar{B} \setminus \bar{A}\}$ is the event lying in the fact that the event \bar{B} occurred and the event \bar{A} did not occur, $\{0\}$ is the impossible event ($P(\{0\}) = 0$)). With account for this relation, we have $P(\bar{B} \setminus \bar{A}) = P(\bar{B}) - P(\bar{B} \cap \bar{A}) = 0$. Thus,

$$P(\bar{B} \cap \bar{A}) = P(\bar{B}). \quad (11)$$

Substituting (11) into (10) and the expression obtained into formula (9) and taking (8) into account, we find

$$P(\overline{B}/\overline{A}) = \frac{P(\overline{A}) - P(\overline{B})}{P(\overline{A})} = \frac{dq}{1-q}. \quad (12)$$

Here it should be noted that the field of events where the calculations were carried out includes both the events occurring with the bond selected for the part of the conducting bonds q and events occurring with the same bond for $q + dq$.

3. Derivation of a System of Differential Equations for a Number of Finite Clusters. As follows from Eq. (12), the probability of transition of the arbitrary nonconducting element to a conducting element is proportional to the small quantity dq . Dealing with the mechanisms of cluster transformation, we will not take into consideration the processes in which two or more bonds of the system become conducting "simultaneously," since the probability of such processes is a quantity of higher order of smallness in dq due to the independence of the properties of different bonds. In the kinetic theory it is analogous to taking account of just paired molecular collisions.

We will consider k -clusters, i.e., clusters containing k sites. When account is taken the processes of just first order in dq , two different methods of formation of new clusters exist.

The first method. A cluster is formed of two clusters of smaller size by their joining. Here two clusters were separated each from other at a certain site by just one nonconducting bond which became conducting with infinitesimal change dq in the system.

Let the part of the conducting bonds in the lattice consisting of N bonds be equal to q . With the infinitesimal increase dq in the part of the conducting bonds the mean number of newly formed clusters of a particular kind in the system can be obtained in the following way. We consider two ensembles of percolation systems with the part of the conducting bonds q (ensemble $\{q\}$) and with the part of the conducting bonds $q + dq$ (ensembles $\{q + dq\}$). Looking over all N bonds of the lattice successively, we will determine their properties (mean with respect to the subensemble). We consider that the k -cluster was formed on an arbitrary bond of the system if the following set of conditions was fulfilled: the given bond was nonconducting with the part of the conducting elements q ; one of the sites belonging to this bond was "wetted" by the k_1 -cluster and the other by the k_2 -cluster (by clusters such that $k_1 + k_2 = k$); with increase in the part of the conducting bonds, the bond considered became conducting (from the viewpoint discussed in Sec. 2. Moreover, it is necessary to take into account the following circumstances. First, two given clusters placed in neighboring sites of the bond considered should not intersect anywhere. Second, they should not intersect any third cluster.

We introduce a combinatorial function by means of which we will try to take into account the above circumstances. We determine this function as the number of mutual arrangements of the given two clusters at two neighboring sites of the considered lattice averaged over all sites of these clusters when the clusters do not intersect. The following relation can be written for the function introduced:

$$g(k_1, k_2, q) = \langle g_{12} \rangle_{k_1 k_2} (1-q)^{z k_1} (1-q)^{z k_2}. \quad (13)$$

Here $\langle g_{12} \rangle_{k_1 k_2}$ is the site-average number of mutual arrangements of the k_1 - and k_2 -clusters for situations where the clusters do not intersect; $(1-q)^{z k_1}$ and $(1-q)^{z k_2}$ are the probabilities that the cluster containing k_1 or k_2 sites, respectively, and being placed in the site selected will not intersect any third cluster; $(1-q)^z$ is the probability that an arbitrary site of the lattice with coordination number z is not wetted). It should be noted that the quantities $\langle g_{12} \rangle_{k_1 k_2}$ for any pair of finite clusters depend on the configuration of the given clusters and the lattice type but not on q .

The following expression can be written for the number of elementary events favorable for the formation of the k -cluster by the first method:

$$\begin{aligned}
 N_k^{(1+)}(q) &= 2NP(B/\bar{A}) \sum_{\{k_1+k_2=k\}} \left(\langle g_{12} \rangle_{k_1 k_2} (1-q)^{(k_1+k_2)z} k_1 n_{k_1}(q) k_2 n_{k_2}(q) \right) = \\
 &= dq 2N (1-q)^{kz-1} \sum_{\{k_1+k_2=k\}} \left(\langle g_{12} \rangle_{k_1 k_2} k_1 n_{k_1}(q) k_2 n_{k_2}(q) \right). \tag{14}
 \end{aligned}$$

Here N is the number of bonds equal to the number of conducted tests; $k_1 n_{k_1}(q)$ and $k_2 n_{k_2}(q)$ are the probabilities that the sites of an arbitrary bond belong to the k_1 - or k_2 -cluster, respectively; $P(B/\bar{A})$ is the probability of transition of the nonconducting element to a conducting element with infinitesimal change in the system. The coefficient equal to two occurs because it makes no difference precisely which of the two sites is wetted and by which cluster (i.e., there is definite symmetry in the problem). The probability that the bond tested is nonconducting is included implicitly in the quantities $(1-q)^{zk_1}$ and $(1-q)^{zk_2}$. These multipliers occur in the equation due to the requirement according to which the k_1 - and k_2 -clusters placed in the sites of the bond tested should not intersect any third cluster. This condition already involves the requirement of "nonwettability" of the sites of the bond tested for q . However, the sites are not wetted only in the case where all the bonds adjoining them *and consequently the bond considered* are nonconducting. Thus, it is seen that multiplication of the entire expression by $(1-q)$, i.e., by the part of the nonconducting bonds in the system, would lead to a twofold account for this circumstance. We note that all the probabilities can be multiplied due to the independence of the properties of any element of the percolation system on the properties of neighboring elements.

The second method. In this case, the k -cluster is formed of the $(k-1)$ -cluster. This occurs when one of the nonconducting bonds forming the perimeter of a smaller cluster becomes conducting with the infinitesimal change dq in the system.

Now the scheme of arguments is analogous to that preceding formula (14). Then we can write the following expression for the number of elementary events favorable for the formation of the k -cluster by the second method:

$$N_k^{(2+)}(q) = 2N P(B/\bar{A}) (k-1) n_{k-1} (1-q)^z = dq 2N (k-1) n_{k-1} (1-q)^{z-1}. \tag{15}$$

Here all the quantities are analogous to ones considered in formula (14); $(1-q)^z$ is the probability that the site is not wetted. In this instance, the probability that the bond considered is nonconducting is included implicitly in the quantity $(1-q)^z$ since a site is not wetted only in the case where all the bonds adjacent to it (and consequently the given bond) are nonconducting.

Next, it is appropriate to note that all the finite clusters can both be formed of clusters of smaller size and disappear, transforming to clusters of larger size.

With account for the fact that in the system an infinite cluster can exist, three different mechanisms of "disappearance" of any finite cluster occur. Two of them are analogous to the above situations of the formation of new clusters with the only difference being that the cluster considered must necessarily appear as one of the clusters involved in the process and any finite cluster can serve as the second. The essence of the third mechanism is that the number of k -clusters can, in addition, decrease, because they will join an IC.

We write the following expressions for the number of elementary events favorable for the disappearance of the k -cluster by the first and second methods, respectively:

$$\begin{aligned}
N_k^{(1-)}(q) &= 2NP(\overline{B/A}) \sum_{k_3=2}^{\infty} \left(\langle g_{12} \rangle_{kk_3} (1-q)^{(k+k_3)z} kn_k(q) k_3 n_{k_3}(q) \right) = \\
&= dq 2N kn_k(q) (1-q)^{kz} \sum_{k_3=2}^{\infty} \left(\langle g_{12} \rangle_{kk_3} (1-q)^{k_3z-1} k_3 n_{k_3}(q) \right), \tag{16}
\end{aligned}$$

$$N_k^{(2-)}(q) = 2NP(\overline{B/A}) kn_k (1-q)^z = dq 2N kn_k(q) (1-q)^{z-1}. \tag{17}$$

According to the scheme of arguments analogous to the previous cases, we write the following expression for the number of elementary events in which the k -cluster can join an IC:

$$N_k^{(3-)} = 2NP(\overline{B/A}) g(k, q) kn_k(q) Q_p(q) = dq 2N \frac{g(k, q) kn_k(q) Q_p(q)}{1-q}. \tag{18}$$

Here $g(k, q)$ is the combinatorial function for the finite and infinite clusters. We determine this function, just as in the case of two finite clusters, as the number of mutual arrangements of the two clusters averaged over all sites of the clusters for situations where the given clusters do not intersect each other and any third cluster. Two circumstances should be noted. First, the number of mutual arrangements of the finite and infinite clusters at the sites of the selected bond depends on q both due to the change in the number of finite clusters near the IC boundary with change in q and because of the change in the IC geometry (and consequently in the number of possible mutual arrangements of the two clusters) as the part of the conducting bonds increases. Second, the percolation-system model used has a special feature. We stated that the system consists of N elements (N is the macroscopic number). Consequently, the system has a certain boundary (even in the thermodynamic limit $N \rightarrow \infty$) to which $\sim N^{1/d}$ elements belong (d is the dimension of space). In the case $q \rightarrow 1$, the IC boundary will tend to the given boundary. A situation is possible where there will be "no room" for the finite cluster (which will be beyond the system) to "stick to" the infinite cluster but other limitations will be absent. This circumstance can be taken into account in the following way. We extend the lattice mentally to infinity and call this new section the passive lattice. If in calculating the number of possible mutual arrangements of the finite and infinite clusters it turns out that the finite cluster should be placed partly on the passive section of the lattice, we will not reject this combination. It is obvious that all this can be taken into account only in $g(k, q)$. Then we have

$$g(k, q) = g_0(k, q) + g_1(k, q) (1-q)^{kz}, \tag{19}$$

where $g_1(k, q)$ is the average-over-all-sites number of mutual arrangements of the finite and infinite clusters, for situations where the clusters do not intersect each other (without taking account of the boundary effect described); $g_0(k, q)$ has the same meaning as $g_1(k, q)$ with the only difference being that this quantity takes account of just the combinations where the finite cluster arrives at the passive section of the lattice (i.e., $g_0(k, q)$ is responsible for the above boundary effect); $(1-q)^{kz}$ is the probability that the k -cluster will nowhere intersect any third cluster. The possibility that the bond tested is nonconducting is present implicitly in the second term of this expression. In deriving formula (14), we discussed the manner in which this occurs.

We note that the effect described occurs with all values $q \geq q_c$ but in the range $q \rightarrow 1$ it turns out to be dominating.

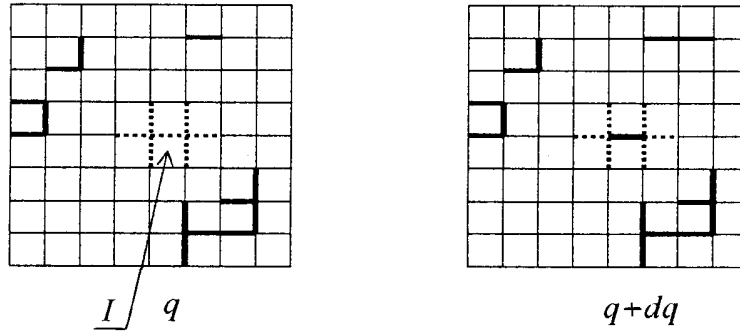


Fig. 1. Scheme of formation of a cluster of minimum size, I is the considered group of bonds.

Now, after stating the most important details and obtaining all the necessary quantities we can write the following balance relation:

$$\frac{2Nn_k(q+dq)}{z} = \frac{2Nn_k(q)}{z} + N_k^{(1+)} + N_k^{(2+)} - N_k^{(1-)} - N_k^{(2-)} - N_k^{(3-)}, \quad (20)$$

where $2N/z$ is the total number of sites in the lattice of N bonds. After simple mathematical transformations, substitution of formulas (14)–(18) into (20) yields the equation sought:

$$\begin{aligned} \frac{dn_k(q)}{dq} = & z(1-q)^{kz-1} \sum_{\{k_1+k_2=k\}} \left(\langle g_{12} \rangle_{k_1 k_2} k_1 n_{k_1}(q) k_2 n_{k_2}(q) \right) + z(1-q)^{z-1} (k-1) n_{k-1}(q) - \\ & - zkn_k(q) \left[(1-q)^{kz} \sum_{k_3=2}^{\infty} \left(\langle g_{12} \rangle_{kk_3} (1-q)^{k_3 z-1} k_3 n_{k_3}(q) \right) + (1-q)^{z-1} + g(k, q) \frac{Q_p(q)}{1-q} \right]. \end{aligned} \quad (21)$$

The question of the equation for the number of minimum-size clusters requires special consideration, since such clusters can be formed by none of the above methods.

Let a part of the conducting elements in the system be equal to q . We consider a group of $2(z-1)$ bonds of the lattice which are adjoining two neighboring sites of this lattice (Fig. 1). For the formation of a minimum-size cluster with increase in the part of the conducting elements, it is necessary that both sites be not wetted for the part of the conducting elements q and the bond connecting the sites considered should become conducting with increase in q . All the other bonds of the group must remain nonconducting.

It can be shown that the expression for the number of elementary events favorable for the formation of a minimum-size cluster has the form

$$N_2^{(+)}(q) = NP(\overline{B/\overline{A}}) (1-q)^z (1-q)^z = dqN(1-q)^{2z-1}. \quad (22)$$

In this case it is not necessary to take account of commutation symmetry, since both sites must have the same property.

Using the same manipulations as in deriving Eq. (21), we obtain the following equation for the number of minimum-size clusters:

$$\frac{dn_2(q)}{dq} = \frac{z}{2} (1-q)^{2z-1} - z2n_2(q) \times$$

$$\times \left[(1-q)^{2z} \sum_{k_3=2}^{\infty} \left(\langle g_{12} \rangle_{2k_3} (1-q)^{k_3 z - 1} k_3 n_{k_3}(q) \right) + (1-q)^{z-1} + g(2, q) \frac{Q_p(q)}{1-q} \right]. \quad (23)$$

Thus, the system of "kinetic" (by formal analogy with the molecular kinetic theory) equations (21) and (23) for the number of finite clusters has been obtained, and it should be supplemented with the boundary conditions

$$n_k(0) = 0. \quad (24)$$

The system is not closed due to the presence of the quantities $Q_p(q)$ and g , which are as yet unknown. The "macroscopic" function $Q_p(q)$ can be expressed in terms of $\{n_k(q)\}$ using formula (5). At this stage of investigation, only some qualitative considerations can be applied to the behavior of the quantities g .

4. Approximate Solution of the System of Equations for the Number of Finite Clusters in Two Limiting Cases. An exact solution of the system obtained is very difficult for several reasons, mainly because of the complexity of calculating the quantities g in the general case. Therefore, we make some assumptions to find an approximate solution of the obtained system of equations for two limiting cases. Then we carry out a qualitative comparison of the solutions obtained to the known analytical expressions.

At first, let us consider the limiting case $q \rightarrow 0$. Then $Q_p(q) = 0$. In addition, all $n_k(q)$ are small quantities in the vicinity of zero due to the boundary conditions (24). Having estimated the order of magnitudes, we arrive at the conclusion that the sum on the square brackets on the right-hand sides of Eqs. (21) and (23) can be neglected as compared to $(1-q)^{z-1}$ in the limit $q \rightarrow 0$ when the condition $q \ll \left(\frac{4}{z^2(z-1)} \right)^{\frac{1}{2+k}} \leq \left(\frac{4}{z^2(z-1)} \right)^{\frac{1}{4}}$ is fulfilled. Then system (21), (23) takes the following form:

$$\frac{dn_2(q)}{dq} \approx \frac{z}{2} (1-q)^{2z-1} - z 2n_2(q) (1-q)^{z-1}, \quad (25)$$

$$\begin{aligned} \frac{dn_k(q)}{dq} \approx z (1-q)^{kz-1} \sum_{\{k_1+k_2=k\}} \left(\langle g_{12} \rangle_{k_1 k_2} k_1 n_{k_1}(q) k_2 n_{k_2}(q) \right) + z (1-q)^{z-1} (k-1) n_{k-1}(q) - \\ - z k n_k(q) (1-q)^{z-1}. \end{aligned} \quad (26)$$

After approximate integration of system (25), (26) with account for the boundary conditions (24) the solution can be represented by the following way:

$$n_2(q) = \frac{z}{2} q (1-q)^{2(z-1)} + \frac{z}{2} \sum_{m=1}^{\infty} \alpha_m^{(2)} q^m; \quad n_k(q) = \frac{z}{2} a'_k q^i (1-q)^j + \frac{z}{2} \sum_{m=1}^{\infty} \alpha_m^{(k)} q^m, \quad (27)$$

where $i = k-1$, $j = k(z-2) + 2$, and $\alpha_m^{(k)}$ and a'_k are some numerical coefficients (for example, $\alpha_1^{(2)} = 0$, $\alpha_2^{(2)} = -4z + 1/2$, ...). The given solution correlates well with expression (2), which holds for $n_k(q)$ in the general case. The presence of additional terms in Eq. (27) is related to the approximate character of the solution. We note that one of the problems of this work is finding the coefficients a'_k with the aim of using further the solution obtained in a number of practical applications. This will be done below.

Let us consider the second limiting case $q \rightarrow 1$. A significant distinction of this situation is that now there is an infinite cluster in the system (one would expect that the influence of the cluster on the properties of the system is dominating). Analysis of system (21), (23) shows that in this limit only the term responsible for the interaction of the finite and infinite clusters can be left in the square brackets on the right-hand sides of the equations, while the other terms can be neglected in the first approximation. In the given limit, we also suppose that the finite cluster with a degree of probability will not meet another finite cluster near the system boundary. Therefore $g_0(k, q)$ in Eq. (19) will be considered to be independent of q in the first approximation, i.e., $g_0(k, q) \approx g_0(k_0)$. Then upon substitution of expressions (5) and (19) and with account for the fact that in the given limit the quantity $(1 - q)$ is a small parameter, we have

$$\frac{dn_2(q)}{dq} \approx \frac{z}{2} (1 - q)^{2z-1} - z 2n_2(q) \frac{g_0(2)}{1 - q}, \quad (28)$$

$$\begin{aligned} \frac{dn_k(q)}{dq} \approx z (1 - q)^{kz-1} \sum_{\{k_1+k_2=k\}} \left(\langle g_{12} \rangle_{k_1 k_2} k_1 n_{k_1}(q) k_2 n_{k_2}(q) \right) + z (1 - q)^{z-1} (k - 1) n_{k-1}(q) - \\ - z k n_k(q) \frac{g_0(k)}{1 - q}. \end{aligned} \quad (29)$$

The general solution of Eq. (28) has the following form:

$$n_2(q) = (1 - q)^{2zg_0} \left[C + \frac{z}{2} \int_1^q (1 - t)^{2z-1-2zg_0} dt \right]. \quad (30)$$

Equation (28) is a linear nonhomogeneous differential equation with singular point $q = 1$ (nodal singularity). This means that the uniqueness of the solution of the considered Cauchy problem is disturbed breaks down at the point $q = 1$. Out of the set of solutions of this equation, passing through the indicated point, we select one from the following consideration: the solution must tend to the form (2) in the limit $q \rightarrow 1$. For this purpose, it is necessary to set $C = z/2$, $2zg_0(2) = j_2$, where $j_2 = 2(z - 1)$ is the perimeter of the cluster consisting of two sites. Then from Eq. (30) we obtain

$$n_2(q) = \frac{z}{2} (2 - q) q (1 - q)^{j_2} \cong \frac{z}{2} q (1 - q)^{j_2}. \quad (31)$$

We note that in the general case the relation $kzg_0(k) = j_k^{(\min)}$ is a consequence of analogous considerations.

Using the mathematical-induction method, we can show that number of clusters of any size, as the solution of Eqs. (28) and (29) in the limit $q \rightarrow 1$, will be determined by the following formula:

$$n_k(q) = \frac{z}{2} a_k q^{i_k} (1 - q)^{j_k} + o((1 - q)^{j_k}). \quad (32)$$

Here i_k and j_k are the minimum possible size and perimeter, respectively, of the k -cluster. We note that these minimum characteristics in the general case can be realized on various (i, j) -clusters. The latter means that

Eq. (32) in the general case characterizes not the relative number of some concrete (i, j) -clusters but just the mean density of the k -clusters in the region of high saturation.

Using Eqs. (21) and (32), we will try to find the coefficients a_k (the coefficient $a_2 = 1$ has actually been obtained already in (31)). For this purpose, we substitute (32) into (21), expanding the percolation probability in a Taylor series in q . This assumption means that our considerations are valid far off the percolation threshold. Next we transpose all the terms to the left-hand side of the equation. On the basis of the uniqueness of a power series, the coefficients for each power of q must be equal to zero each by itself. We consider the first two coefficients for the lowest powers of q , namely, for $q^{i_k^{(\min)}-1}$ and $q^{i_k^{(\min)}}$. Then we have

$$i_k a_k - z \sum_{\{k_1+k_2=k\}} \left(\langle g_{12} \rangle_{k_1 k_2} k_1 a_{k_1} k_2 a_{k_2} \right) - z (k-1) a_{k-1} = 0, \quad (33)$$

$$i_k a_k (j_k + 1) + j_k a_k - z \sum_{\{k_1+k_2=k\}} \left(\langle g_{12} \rangle_{k_1 k_2} k_1 a_{k_1} k_2 a_{k_2} (j_{k_1} + j_{k_2} + kz) \right) - z (k-1) a_{k-1} (j_{k-1} + z - 1) - z k a_k = 0. \quad (34)$$

We could obtain the recurrence relation for the coefficients a_k only from Eq. (33). However, in this case they will be expressed in terms of the quantities $\langle g_{12} \rangle_{k_1 k_2}$, whose calculation is as complex as that of a_k . Thus, we will try to eliminate the quantities $\langle g_{12} \rangle_{k_1 k_2}$ from consideration using Eq. (34). For this purpose, we perform the following transformation:

$$j_{k_1} + j_{k_2} + kz = k_1 z - 2i_{k_1} + k_2 z - 2i_{k_2} + kz = (k_1 + k_2) z - 2(i_{k_1} + i_{k_2}) + kz = \\ = \left\{ k_1 + k_2 = k, i_{k_1} + i_{k_2} = i'_k - 1 \right\} = kz - 2i'_k + kz + 2 = 2(kz + 1 - i'_k). \quad (35)$$

Here i'_k is the size of the k -cluster formed of the (i_{k_1}, j_{k_1}) - and (i_{k_2}, j_{k_2}) -clusters. The problem lies in the fact that the value of i'_k is not fixed ($i_k^{(\min)} \leq i'_k \leq i_k^{(\max)}$). Therefore, we assume that

$$i'_k \approx \frac{i_k^{(\min)} + i_k^{(\max)}}{2}. \quad (36)$$

If we now substitute (36) into (35), expression (35) can be taken outside the summation sign in (34). Then all the coefficients $\langle g_{12} \rangle_{k_1 k_2}$ in (33) and (34) will be involved in the same sum. Having eliminated this sum from the two equations, upon simple transformations we obtain the following expression for a_k :

$$a_k = z (k-1) a_{k-1} \frac{k(z-1) + 4 + 2i_{k-1}^{(\max)} - i_k^{(\max)}}{(k-1)[k(z-1) + 2 + i_k^{(\max)}] + 2i_k^{(\max)}}. \quad (37)$$

Formula (37) gives the value $a_3 = z(3z+1)/(3z+3)$, whereas the exact value is $a_3 = z-1$ (the coefficients a_k for small k can be found directly). Equation (37) gives a somewhat larger value for a_4 in comparison to the exact one. We construct a plot for the quantity ka_k on a logarithmic scale for verification of formula (37) for large k . As can be seen from Fig. 2, the linear dependence of the logarithm of ka_k on k occurs for all the lattices. This result is in qualitative agreement with the results of [15].

Thus, we have shown that in two limiting cases the obtained system of equations for the number of finite clusters had solutions conforming to formula (2), which holds for $n_k(q)$ in the general case. As we have

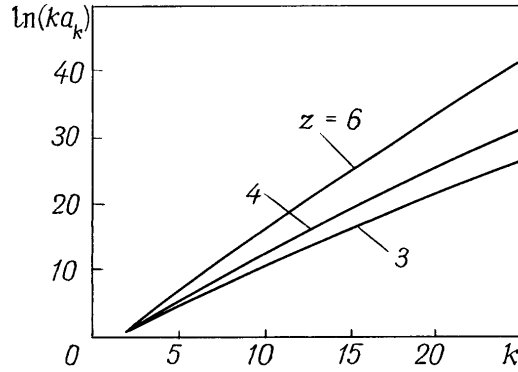


Fig. 2. Dependence of the logarithm of ka_k on k for three different lattices: simple cubic ($z = 6$), square ($z = 4$), and honeycomb ($z = 3$).

already assured ourselves, the given system is rather complex, and obtaining its exact solution seems impossible for a variety of reasons. We suppose that the basic application of this system will be related to a qualitative analysis of the behavior of the percolation system over the entire range of variation in q and to its quantitative description in a number of limiting cases.

5. Equation for the Percolation Probability. The approach developed can be applied directly to an infinite cluster whose basic characteristics ($Q_p(q)$, $Q_b(q)$, and $S_{IC}(q)$) are related to $n_k(q)$.

After carrying out some calculations, we will show that knowledge of just one characteristic of the IC (for example, of the percolation probability $Q_p(q)$) will enable one to find all the basic characteristics of the IC.

We establish the relation between the connectivity function $Q_b(q)$ and the percolation probability $Q_p(q)$, i.e., between the part of the bonds and the part of the sites of the system that belong to the infinite cluster.

Let us consider the set of conditions under which an arbitrary site of lattice can belong to the IC. The event B_l will be assumed to occur on an arbitrary site of the lattice if any l of z bonds adjoining the given site belong to the IC and the other $(z-l)$ bonds are nonconducting ($l = 1, \dots, z$). The events B_l are independent in pairs. The given site belongs to the IC (the event D) if any of the events B_l occurred. Then we can use the formula of total probability:

$$Q_p(q) = P(D) = \sum_{l=1}^z P(B_l) P(D/B_l). \quad (38)$$

According to the above, we have the following relations:

$$P(D/B_l) = 1, \quad P(B_l) = C_z^l [Q_b(q)]^l (1-q)^{z-l}, \quad l = 1, \dots, z, \quad (39)$$

where C_z^l is the number of combinations from z by l .

Substituting (39) into (38), we can finally write

$$Q_p(q) = \sum_{l=1}^z C_z^l [Q_b(q)]^l (1-q)^{z-l} = \{1 - [q - Q_b(q)]\}^z - (1-q)^z. \quad (40)$$

According to the analogous scheme of arguments concerning the membership of an arbitrary site in the perimeter of the IC, we obtain the following expression:

$$S_{IC}(q) = 2(1-q) \{ [1-q+Q_b(q)]^{z-1} - (1-q)^{z-1} \}. \quad (41)$$

Now, to determine three quantities characterizing the IC, namely, the numbers of sites $Q_p(q)$, the numbers of bonds $Q_b(q)$ entering into the IC, and the cluster perimeter $S_{IC}(q)$, it will suffice to find one of them and then the other two can be obtained by means of relations (40) and (41).

From the viewpoint of our approach, the derivation of a differential equation for the percolation probability $Q_p(q)$ and its subsequent solution are best suited. Now we turn to just this procedure.

It was proved in consideration of the problem of the number of an IC [14] that it was equal to $n_\infty = 0, 1$ or ∞ , where the values presented correspond to the absence of percolation, its presence, and the Bethe lattices only, respectively. As has already been noted, we consider problems of percolation theory for regular lattices, i.e., in our case $n_\infty = 0$ or 1 .

We emphasize in particular that in the process of increase in the part of the conducting elements, an increase in the part of the sites belonging to the IC and not the formation of new ICs will occur.

With account for the processes of only first order in dq , there are two different mechanisms of increase in the IC density for a regular lattice, namely, joining of an arbitrary finite cluster and joining of one of the sites along the IC perimeter.

A situation analogous to that discussed in deriving Eq. (18) is observed in the process of joining of the finite and infinite clusters. In this case, when one more k -cluster joins the IC, an increase in the IC density occurs:

$$\Delta_k^{(1)} Q_p = z \frac{k}{2N}. \quad (42)$$

Then the increase in the IC density due to the interaction of the IC with the finite clusters for the infinitesimal change dq in the system will be as follows:

$$\Delta^{(1)} Q_p(q) = 2 \sum_{|k|} \left\{ z \frac{k}{2N} NP(B/\bar{A}) kn_k(q) Q_p(q) g(k, q) \right\} = dq \frac{zQ_p(q)}{1-q} \sum_{|k|} k^2 n_k(q) g(k, q), \quad (43)$$

where N is the number of bonds equal to the number of tests performed; kn_k is the probability of the given site belonging to the k -cluster determined by formula (3); $Q_p(q)$ is the probability of the other site belonging to the IC; $g(k, q)$ is the combinatorial function for the finite and infinite clusters determined by Eq. (19); the summation is carried out over all the finite clusters. The coefficient in front of the sum in Eq. (43), equal to two, arises due to the commutation symmetry which occurs in this case and has been discussed earlier.

The essence of the second mechanism of increase in the IC density is as follows: the IC density can also increase in the case where one of the nonconducting bonds forming the IC perimeter becomes conducting (just one site joins the IC).

In this case, the IC density changes by $z/(2N)$ in an elementary process. Here the increase of the IC density with for the infinitesimal change dq in the system will be as follows:

$$\Delta^{(2)} Q_p(q) = 2 \frac{z}{2N} N (1-q)^z P(B/\bar{A}) Q_p(q) = dq z Q_p(q) (1-q)^{z-1}, \quad (44)$$

where $(1-q)^z$ is the probability of isolation of the site.

Next we write the relation

$$Q_p(q+dq) = Q_p(q) + \Delta^{(1)} Q_p(q) + \Delta^{(2)} Q_p(q). \quad (45)$$

Using expressions (43) and (44), after simple transformations we obtain the following differential equation:

$$\frac{dQ_p}{dq} = zQ_p(q) \left[\sum k^2 n_k(q) \frac{g(k, q)}{1-q} + (1-q)^{z-1} \right], \quad q_c \leq q \leq 1. \quad (46)$$

This is precisely the equation for the percolation probability Q_p . It is open since the quantities $n_k(q)$ and the combinatorial function $g(k, q)$ are involved in it. It should be noted that the obtained system of equations for the number of the finite clusters $n_k(q)$ can be used for the process of closure of Eq. (46). However, with such an approach we run into the same problems, which because of we were unable to solve exactly the system of equations for finite clusters. Therefore, we propose below the method of approximate closure of Eq. (46).

6. Approximate Solution of the Equation for the Percolation Probability in Two Limiting Cases.

First of all, we consider the case $q \rightarrow 1$. Let us estimate the relation between the sum and the second term in Eq. (46) in this limit. We keep only the first term of the sum as essential in this limit. Then, with account for Eqs. (31), (32), and (36), we have

$$\left[\sum k^2 n_k(q) \frac{g(k, q)}{1-q} \right] \Big/ \left[(1-q)^{z-1} \right] \approx 2z(z-1)q(1-q)^{z-2}.$$

That is why the sum in (46) in the limit $q \rightarrow 1$ can be neglected. As a result, we obtain the following equation:

$$\frac{dQ_p}{dq} \approx zQ_p(q) (1-q)^{z-1},$$

under the boundary condition $Q_p(1) = 1$ the following relation is obtained:

$$Q_p(q) = \exp \left[- (1-q)^z \right] \cong 1 - (1-q)^z, \quad (47)$$

which is in good agreement with formula (5) for $q \rightarrow 1$.

The vicinity of the percolation threshold ($q \rightarrow q_c$) is of greatest interest to us.

According to present-day concepts, the occurrence of the IC is caused by large-scale fluctuations in the system and is the phase transition of the second kind [5, 19]. The correlation length, which is introduced in percolation theory by the standard method [14], tends to infinity in the percolation threshold. This means that the basic macroscopic parameters of the system in the vicinity of the percolation threshold become independent of some space characteristics. In this case, it is important to us that such small-scale properties of the system as the arrangement of finite clusters have no substantial effect on the behavior of the system. Then we assume relative to the behavior of the combinatorial function in this range of values of q that correlations of the finite clusters and the infinite one in the vicinity of the percolation threshold are determined, first of all, by the structure of the infinite cluster and turn out to be insensitive to the properties of the finite clusters. This means that $g(k, q)$ can be represented in the given range as

$$g(k, q) = \bar{g}(q). \quad (48)$$

To obtain the correct result, it is necessary to take explicit account of the properties of the bond tested, namely, to set

$$\bar{g}(q) = (1-q) \bar{\bar{g}}(q). \quad (49)$$

Since, in the percolation threshold itself, the IC occurs for the first time (until this moment it did not exist in the system), the following relation must be fulfilled:

$$\lim_{q \rightarrow q_c^+0} g(k, q) = 0. \quad (50)$$

We suppose that tending to zero in Eq. (50) will follow the power law:

$$\bar{g}(q) = g'_0 |q - q_c|^\lambda, \quad \lambda \geq 0, \quad (51)$$

where g'_0 and λ are some quantities independent of q . This assumption is based on the concept prevalent in the theory of phase transitions of the second kind (which can include the occurrence of the IC) that consists of the fact that the behavior of the thermodynamic functions near the phase-transition point is described by simple power functions [20].

Equation (46) with account for (5), (7), and (48)–(51) takes the following form in the vicinity of the percolation threshold:

$$\frac{dQ_p(q)}{dq} = zQ_p(q) \left[g'_0 |q - q_c|^\lambda S(q) \left(1 - (1 - q)^z - Q_p(q) \right) + (1 - q)^{z-1} \right]. \quad (52)$$

Well established and repeatedly proved (see, for example, [14, 21]) is the fact that the mean size of the finite clusters $S(q)$ in the vicinity of the percolation threshold behaves as follows:

$$S(q) \approx s_0 |q - q_c|^{-\gamma}. \quad (53)$$

Substitution of (53) into (52) results in

$$\frac{dQ_p}{dq} = zQ_p(q) \left[g'_0 s_0 |q - q_c|^{\lambda-\gamma} \left(1 - (1 - q)^z - Q_p(q) \right) + (1 - q)^{z-1} \right]. \quad (54)$$

The percolation probability near the percolation threshold is a small quantity. Therefore, we consider an approximation of Eq. (54) linear in $Q_p(q)$:

$$\frac{dQ_p}{dq} \approx zQ_p(q) \left[g'_0 s_0 |q - q_c|^{\lambda-\gamma} \left(1 - (1 - q)^z \right) + (1 - q)^{z-1} \right]. \quad (55)$$

Analysis of this equation showed that it has three qualitatively different solutions corresponding to the cases $\lambda < \gamma - 1$, $\lambda = \gamma - 1$, and $\lambda > \gamma - 1$. The solution which is correct physically is obtained only with $\lambda = \gamma - 1$.

Based on highly general considerations, it can be shown that the point of the phase transition of the second kind has a singularity of the saddle type [22]. In our case this situation occurs, too.

The general solution of Eq. (55) with $\lambda = \gamma - 1$ is of the form

$$Q_p(q) = C |q - q_c|^{\tau_1} \exp \left[\sum_{n=1}^z \left(\sum_{i=1}^n b_{ni} (q - q_c)^i \right) + (1 - q_c)^z - (1 - q)^z \right], \quad (56)$$

where C is the integration constant; $\tau_1 = \frac{z g'_0 s_0}{1 - q_c} [1 - (1 - q_c)^z]$; $b_{ni} = \frac{(-1)^{n+1} z! (q_c)^{n-i}}{i(z-n)!(n-i)!}$.

For Eq. (56) to be in agreement with the known scaling relations (see, for example, [14]), it is necessary to set $\tau_1 = \beta$.

TABLE 1. Maximum Number of Bonds $i_k^{(\max)}$ Entering into the k -Cluster for the Case of a Simple Cubic Lattice ($z = 6$)

k	2	3	4	5	6	7	8	9	10	11	12	13
$i_k^{(\max)}$	1	2	4	5	7	9	12	13	15	17	20	21
k	14	15	16	17	18	19	20	21	22	23	24	25
$i_k^{(\max)}$	23	25	28	30	33	34	36	38	41	43	46	48

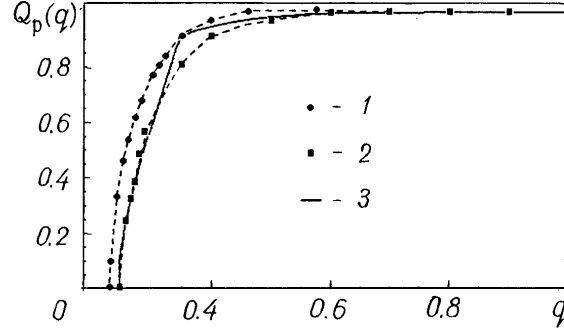


Fig. 3. Percolation probability $Q_p(q)$ for a simple cubic lattice ($z = 6$): 1) numerical experiment [23]; 2) results of numerical experiment [24] recalculated using Eq. (40); 3) calculation from Eqs. (5), (32), (37), and (56).

To obtain expressions for $Q_p(q)$ over the entire range of change in q , we join Eq. (56) with the solution found in the vicinity of unity. The joining with Eq. (47) and the subsequent comparison of the relation obtained to the results of the numerical experiment show that Eq. (47) is still a rather rough approximation. Therefore, we will use the system of equations for the finite clusters in the vicinity of unity, namely, relations (32) and (37) and Eq. (5) in the limit mentioned. This procedure will be carried out for a simple cubic lattice ($z = 6$). The only information which is needed here is the maximum sizes of the clusters $i_k^{(\max)}$. They are presented in Table 1. As it has turned out, it is possible to restrict oneself to the case where $k = 21$ in order to achieve satisfactory accuracy.

The joining results are presented in Fig. 3. In this case, the joining point turned out to be equal to $q^* = 0.3468$, and the constant in Eq. (56) is equal to $C = 2.277$.

Thus, the formula for $Q_p(q)$ takes the following form:

$$Q_p(q) = C |q - q_c|^\beta \exp \left[\sum_{n=1}^z \left(\sum_{i=1}^n b_{ni} (q - q_c)^i \right) + (1 - q_c)^z - (1 - q)^z \right], \quad q_c \leq q \leq q^*; \quad (57)$$

$$Q_p(q) = 1 - (1 - q)^z - \sum_{k=2}^{21} k a_k q^{i_k} (1 - q)^{j_k}, \quad q^* \leq q \leq 1.$$

In conclusion, we note that in [25] an interpolation formula for $Q_p(q)$ has been obtained by joining of the simple asymptotic expression $Q_p(q) \sim (q - q_c)^\beta$ and the expression from [26]. Our result differs in the fact that formula (57) has been obtained within the framework of a unified approach which enables one not only to make quantitative estimates but to carry out qualitative analysis of the behavior of the percolation system as well. Moreover, in our case it is possible to obtain more comprehensive information on the system due to relations (40) and (41).

We also note that most of the results of the work can be extended to the problem of sites practically immediately. Basically, the changes will be related to the notation and definitions.

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CONCLUSIONS

1. For the first time, the system of differential equations (21) and (23) for the number of finite clusters has been derived, which enables one to carry out qualitative analysis of the behavior of the percolation system over the entire range of change in q .

2. The differential equation (46) for the percolation probability $Q_p(q)$ has been obtained. A method of approximate closure of this equation using the system of equations for the number of finite clusters has been developed. Moreover, relations have been found which connect $Q_p(q)$ with other characteristics of the IC: the relative number of bonds $Q_b(q)$ and the cluster perimeter $S_{IC}(q)$.

3. The expressions for the percolation probability for the case of a simple cubic lattice, obtained in two limiting cases, have been compared to the data of numerical experiment [23, 24]. Their satisfactory agreement has been revealed.

NOTATION

q and $(1 - q)$, parts of permeable and impermeable pores in the lattice, respectively; z , coordination number of the lattice; i , number of conducting bonds entering into the cluster; j , cluster perimeter; k , number of sites entering into the cluster; $j_k^{(\min)}$, minimum possible perimeter for the cluster of k sites on the given lattice; $i_k^{(\max)}$ and $i_k^{(\min)}$, maximum and minimum numbers of bonds which can be contained in the cluster of k sites on the given lattice, respectively; $Q_b(q)$, connectivity function or part of the bonds forming the infinite cluster; $F(q)$, part of the bonds belonging to the clusters of finite size; $Q_p(q)$, percolation probability or part of the lattice sites entering into the infinite cluster; $S_f(q)$, perimeter of the finite clusters or number of impermeable pores which limit the finite clusters (the number is referred to N); $S_{IC}(q)$, perimeter of the infinite cluster; $S(q)$, mean size of the finite clusters; q_c , percolation threshold. Subscripts: γ and β , critical indexes of the percolation theory; k , cluster consisting of k sites; ij , (i, j) -cluster; c, critical; p, probability; f, finite; b, bond.

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