Cluster size distribution in percolation theory and fractal Cantor dust

Pavel Grinchuk*

A. V. Luikov Heat and Mass Transfer Institute, National Academy of Sciences of Belarus, 15 Petrus Brovka Str., Minsk 220072, Belarus

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Results of numerical simulation of cluster size distribution in the site percolation problem are presented. These results disagree with the theoretical data obtained on the basis of the standard drop model of finite cluster structure, in particular, they give a different value of exponent ζ ($\ln n_s \sim -s^{\zeta}$). Therefore, a more precise fractal model for describing the structure of clusters in a percolation system is proposed. The consideration is based on the solution of a kinetic equation for the number of finite clusters. In the framework of the proposed approach (fractal model together with kinetic equation), a correct value of exponent ζ is obtained and an explanation is given to the dependence of this exponent on the fraction of occupied sites p, which was revealed by numerical simulations. Additionally, a relation is established between the characteristics of cluster size distribution and fractal dimension of the Cantor dust constructed on the percolation cluster.

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I. INTRODUCTION

Percolation theory has numerous applications in practical and scientific problems. The typical examples are materials science [1–3], nanotechnology [4], optics [5], combustion theory [6], biology [7], social science [8], etc. One of the most-used problem is site percolation. In this problem, random distribution of occupied and empty sites on a lattice is considered. Main properties of the whole system can be described by means of characteristics of this distribution. The occupied sites on the lattice exhibit a tendency to aggregate into clusters. The cluster size distribution $n_s(p)$ is a main characteristic of a percolation system. The function $n_s(p)$ is a discrete analog of the distribution function in statistical physics. Unfortunately, a general analytical solution of this classical problem is not known even for the two-dimensional case, and main results were obtained by numerical simulation or on the basis of the scaling hypothesis.

As is known, all nontrivial properties of considered random systems are associated with the formation of a percolation cluster (PC), which spans over the whole system. This cluster arises at the percolation threshold p_c. The cluster numbers $n_s(p)$ are known exactly for $s \leqslant 10$ [9–11]. Therefore, this problem may be thought as solved for p far from p_c because in this case there is a small amount of large clusters. However, this problem in the neighborhood of the percolation threshold remains unsolved and is of great interest.

One of the most important and, at the same time, scantily known parameters in this region is exponent ζ [12,13]. This exponent describes the behavior of finite clusters in the vicinity of the percolation threshold depending on cluster size s

$$\ln n_s \sim -s^{\zeta}, \quad s \gg 1. \tag{1}$$

Also, this exponent determines the behavior of mean perimeter t_s of finite clusters [13,14]:

$$t_s = s\frac{1-p}{p} + \text{const}\, s^{\zeta}. \tag{2}$$

According to the drop model of cluster structure, for $p > p_c$ on d-dimensional lattice the following expression $\zeta = 1 - 1/d$ is known [12,13]. Unfortunately, this expression for exponent ζ contradicts to both previous [14] and new results of numerical simulations reported below. Moreover, the drop model gives a very rough description for the structure of large clusters in a percolation system. In this paper we show that the application of fractal model to the cluster structure together with a new kinetic approach for the cluster size distribution allows obtaining a correct expression for exponent ζ which gives much better conformity with the numerical data. In addition, the proposed approach allows one to establish a new relationships between exponent ζ and nontrivial fractal properties of the percolation cluster. This relationships will help us to find the cluster size distribution for some other problems of the percolation theory.

II. NUMERICAL EXPERIMENT FOR EXPONENT ζ

The cluster size distribution $n_s(p)$ is defined as a number of clusters containing s occupied sites per one lattice site when the fraction of occupied sites on the lattice is equal to p. According to the scaling hypothesis [13,15], this distribution above the percolation threshold can be represented as

$$n_s(p) = s^{-\tau} f_0(y), \quad y = (p_c - p)s^{\sigma}, \quad f_0(0) = 1. \tag{3}$$

At the same time different corrections to this expression are known [16]:

$$n_s(p) = s^{-\tau}[f_0(y) + s^{-\lambda} f_1(y)]. \tag{4}$$

At fixed p and $s \gg 1$ for cluster size distribution above percolation threshold is justified the following functional dependence [12,13,15,17,18]:

$$n_s(p) \sim s^{-\tau} \exp[-\text{const}(p)s^{\zeta}]. \tag{5}$$

On the basis of expression (5) the magnitude of exponent ζ can be obtained directly from the data of a usual numerical

*Electronic address: gps@hmti.ac.by

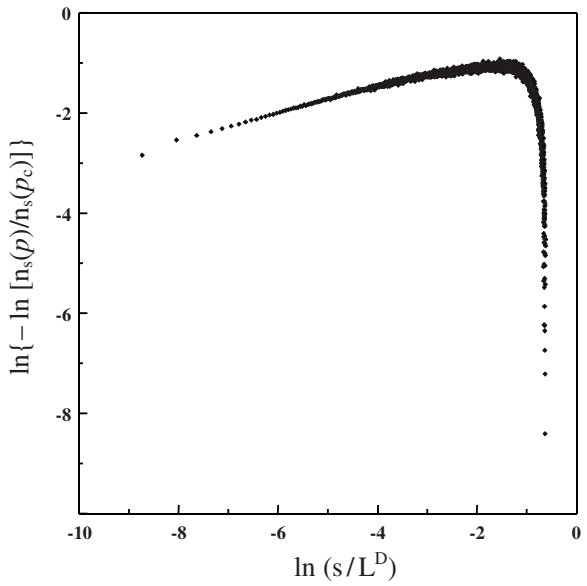

FIG. 1. Cluster size distribution for site percolation on square lattice 100×100 in log-log scale ($p=0.60$, 3×10^7 histories).

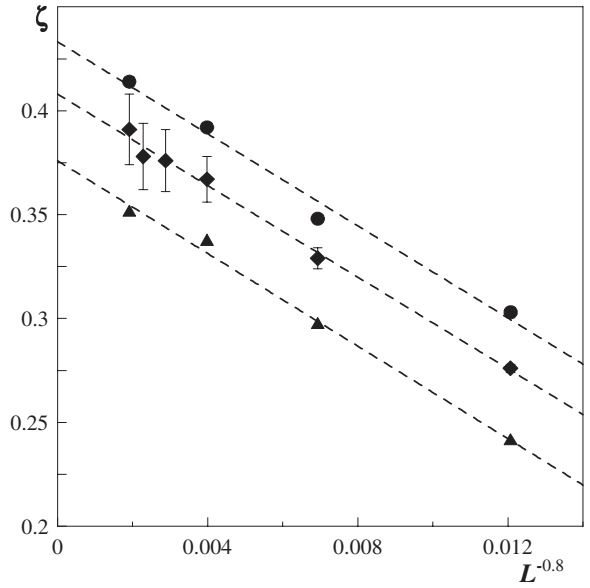

FIG. 2. Exponent ζ vs $L^{-0.8}$ according to numerical experiment. ▲: $p=0.59374621$ ($p-p_c=0.001$), ♦: $p=0.60$, ●: $p=0.61$.

experiment for the site percolation problem. For this purpose we should divide expression (5) by $n_s(p_c)$ [$n_s(p_c)\sim s^{-\tau}$] and twice take the logarithm of the obtained expression. Then in coordinates $\ln(s)$ (abscissa) and $\ln\{-\ln[n_s(p)/n_s(p_c)]\}$ (ordinate) the cluster size distribution will be linear.

We perform a series of Monte Carlo simulations to obtain the cluster size distribution on a square lattice ($p_c=0.59274621$ [19]). All simulations were carried out using the Hoshen-Kopleman algorithm [20]. As can be seen from Fig. 1, in a definite region of cluster sizes such a linear dependence takes place. The magnitude of exponent ζ can be obtained from the slope of this line.

Since a finite lattice was used in the simulations, the size of the system can influence the results [13,21]. Therefore, we carried out simulations for six different sizes of the lattice ranging from 100×100 up to 2500×2500. The cluster size distribution depends on the lattice size L through variable $s/s_{\max}\sim1/L^D$ (here D is the fractal dimension of percolation cluster), because the largest cluster on the lattice contains $s_{\max}\sim L^D$ sites [22]. We took into account this circumstance and used argument s/L^D instead of s. Nevertheless, exponent ζ exhibits a dependence on lattice size L. We found that $\zeta\approx\zeta_\infty+\text{const}\,L^{-0.8}$ to a satisfactory accuracy (Fig. 2). Therefore, exponent ζ_∞ for an infinitely large system can be found from this dependence as a point of intersection with the ordinate axis ($1/L=0$). In such a way, exponent ζ_∞ was found for different fractions of occupied sites p in the vicinity of the percolation threshold (Fig. 2). We found that the considered exponent depends on p: $\zeta_\infty|_{p=0.59374621}=0.37(6)\pm0.02$ ($|p-p_c|=0.001$), $\zeta_\infty|_{p=0.60}=0.40(8)\pm0.02$, $\zeta_\infty|_{p=0.61}=0.43(3)\pm0.02$. The obtained results contradict the conclusions of the traditional drop model. According to this model $\zeta_\infty=0.5$ for square lattice ($d=2$) and is independent of p. These contradictions can be resolved within the framework of the fractal model proposed in this paper.

III. FRACTAL MODEL

In Ref. [17] a kinetic approach to the investigation of cluster size distribution in lattice percolation problems was proposed. For this distribution, a system of kinetic equations was obtained which describes the "diffusion" and "drift" of finite clusters in the space of their sizes when the fraction of occupied sites undergo infinitesimal growth. It should be noted that in Refs. [23,24] a similar approach was proposed for off-lattice percolation problems. In Ref. [17] the mentioned system of equations was applied for investigation of cluster size distribution above the percolation threshold. In particular, it was shown that most of large finite clusters are compact in this region. However, the consideration in Ref. [17] was still based on the drop model of cluster structure.

In this work the same system of kinetic equations for cluster size distribution [17] will be used. But the structure of both the finite clusters and percolation cluster will be described by fractal models.

Thus, the site problem on the square lattice of $N=L^d$ sites is considered. The system of kinetic equations for a number of finite clusters $n_s(p)$ ($s=1,2,3,\ldots$) in this case has the following form [17]:

$$\frac{dn_s(p)}{dp}\approx 2\sum_{s_1+s_2+1=s}[g_{s_1s_2}(p)s_1n_{s_1}(p)s_2n_{s_2}(p)] + 2(1-p)^{z-1}(s-1)n_{s-1}(p) - 2sn_s\left\{\sum_{s_3=1}^{\infty}[g_{ss_3}(p)s_3n_{s_3}(p)] + (1-p)^{z-1} + g(s,p)P(p)\right\}. \quad (6)$$

Here z is the coordination number of a lattice (for a square lattice $z=4$), $P(p)$ is the fraction of sites belonging to the

percolation cluster, $g_{s_1 s_2}$ is a mean number of mutual arrangements of all cluster pairs of sizes s_1 and s_2 at two sites neighboring an arbitrary unoccupied site of the considered lattice when the clusters do not intersect with each other nor with any third cluster; $g(s,p)$ has the same meaning but for the pair "percolation cluster-finite cluster."

Our general assumption allowing the approximate solution of this equations consists in the following: the change in the number of finite clusters above the percolation threshold is determined mainly by the "interaction" of these clusters with the percolation cluster [17]. It means that for determining the cluster size distribution, the following approximate equation will be solved:

$$\frac{dn_s}{dp} \approx -2sn_s(p)g(s,p)P(p), \tag{7}$$

with boundary condition [17]

$$n_s|_{p=p_c} = Cs^{-\tau}. \tag{8}$$

Here τ is the Fisher exponent [13,18], C is a constant independent of s. For the density of a percolation cluster, a well known scaling relation can be used:

$$P(p) \approx C_p(p-p_c)^{\beta}. \tag{9}$$

The main problem consists in the determination of the form of function $g(s,p)$. In our paper [17] it was shown that in the vicinity of percolation threshold

$$g(s,p) \approx g_1(s)g_2(p), \tag{10}$$

where

$$g_2(p) \propto (p-p_c)^{\gamma-1}. \tag{11}$$

In Ref. [17], the governing equation for $g_1(s)$ was also obtained:

$$\frac{dg_1}{ds} \approx \frac{\eta}{s-\eta}g_1(s) - \frac{\theta}{s-\eta}, \tag{12}$$

with boundary condition

$$g_1|_{s=\infty} = 0. \tag{13}$$

Here $\theta=(\Sigma_{m=1}^{s}\theta_m^{(s)})$ is the total decrease in the number of possible allocations of the s cluster in the neighborhood of PC with increasing the size of the former by 1 ($\theta \approx$ const [17]); $\eta=\frac{1}{\Omega}-1$.

The derivation of Eq. (12) is based on the consideration of contribution of each site of a finite cluster and the percolation cluster to function $g_1(s)$. It is important that the sites which are enclosed with occupied sites on all sides (i.e., internal sites of a cluster) will not contribute to function $g_1(s)$.

The key structural parameter in Eq. (12) is Ω. It is defined as the following ratio:

$$\Omega = \frac{s_b}{s}, \tag{14}$$

where s_b is the number of such cluster sites through which finite cluster can be joined to PC without mutual overlapping and intersections.

Let us consider a finite cluster and the percolation cluster as fractal objects. Let R be the characteristic size of a large finite cluster (for example, its gyroradius). Then for the number of sites in this cluster relationship $s \approx \Lambda_1 R^D$ is valid [22], where D is the fractal dimension of the percolation cluster, Λ_1 is a constant. For value s_b a similar expression $s_b \approx \Lambda_2 R^{D_c}$ should be valid where D_c is a fractal dimension of the percolation cluster surface. Then $s_b \approx bs^{D_c/D}$ (where $b=\Lambda_2/\Lambda_1^D$) and for value Ω in the framework of fractal model we have

$$\Omega \approx bs^{D_c/D-1} = bs^{\psi-1}, \tag{15}$$

where

$$\psi = \frac{D_c}{D}. \tag{16}$$

Then Eq. (12) grades into

$$\frac{dg_1(s)}{ds} \approx \frac{bs^{1-\psi}}{s-bs^{1-\psi}}g_1(s) - \frac{\theta}{s-bs^{1-\psi}}. \tag{17}$$

An approximate solution to Eq. (17) with boundary condition (13) follows:

$$g_1(s) \approx \frac{\theta}{1-\psi}[s^{\psi-1} - bs^{-1} + b^2 s^{-1-\psi} + O(s^{-1-2\psi})]. \tag{18}$$

Then for $n_s(p)$ from Eqs. (7), (8), and (18) we have

$$n_s(p) \approx \text{const}\, s^{-\tau}\exp\left(-\frac{s^{\psi}}{s_{\xi}}\right), \tag{19}$$

where

$$s_{\xi} \propto |p-p_c|^{-1/\sigma} \tag{20}$$

is the characteristic size of finite clusters [$\sigma=1/(\gamma+\beta)$] [17].

From the comparison of relationships (5) and (19) we conclude that $\zeta=\psi$, i.e., exponent ζ depends on the fractal properties of the percolation cluster.

At a first sight, fractal dimension D in Eq. (16) should be defined on the whole surface of the percolation cluster, namely it is equal to the fractal dimension of the percolation cluster hull $D_c=D_h$ [25]. For the latter, the following relation $D_h=(\nu+1)/\nu$ is valid [13,25], where ν is the critical exponent of the correlation length. Taking into account that $D=(\gamma+\beta)/\nu$, from Eq. (16) we have $\zeta=(\nu+1)/(\gamma+\beta)$. Then for a 2D system the proposed fractal model gives the value $\zeta \approx 0.93$. This result seems strange: a more precise fractal model gives a larger discrepancy with a numerical experiment ($\zeta \approx 0.4$) as compared with the drop model ($\zeta=0.5$).

The reason for this discrepancy lies in an accurate definition of value s_b [Eq. (14)]. It is a number of such cluster sites through which a finite cluster can be joined to the percolation cluster without mutual overlapping and intersections. The ex-

ternal surface of both a large finite cluster and the percolation cluster is indented and contains many "cavities" and "fjords." The sites inside such fjords should not be taken into account when calculating s_b because inside the fjords may not be enough space for a large cluster. So, the external surface of an arbitrary finite cluster can be considered as a simply connected set (continuous line binding the neighboring sites of surface). However, sites of the both percolation and finite cluster, which contribute to value s_b [i.e., to function $g_1(s)$], represent a multiply connected set because a certain fraction of sites is deleted from the continuous surface. Such a mathematical object is known. It is a Cantor set (or fractal Cantor dust) [22,26]. It is important that the fractal dimension of this set is less than 1.

The one-dimensional Cantor dust C can be constructed in the following way. The initial seed of this set is a unit segment [0, 1]. This segment is divided into three parts. After that the middle part is removed. Each of the residual segments is once again divided into three parts and the middle of them is put away, etc. After infinite number of such iterations the remaining infinite set of points will be scattered over the unit segment. This set is called the Cantor dust. Generally, if a unit segment is divided into three parts, from which two segments with length l_1 and l_2 are left, the fractal dimension D_c of this set will be obtained by solving the following equation [22]:

$$l_1^{D_c} + l_2^{D_c} = 1. \tag{21}$$

So, for example, if $l_1 = l_2 = 1/3$ then $D_c = \ln 2/\ln 3 \approx 0.63$. In the present paper, a two-dimensional problem is considered. The Cantor set can be generalized to the case of two- and multidimensional space [26]. Let us consider a set of points inside a unit square. For all points of this set, both abscissa x and ordinate y belong to a one-dimensional Cantor set C. The Cartesian product $C \times C$ of the Cantor set on itself represents the Cantor dust imbedded in two-dimensional space. The fractal dimension of product of k Cantor sets is equal to

$$D_c(\underbrace{C \times C \times \cdots \times C}_{k \text{ times}}) = kD_c(C). \tag{22}$$

Thus, for exponent ζ we can write the following expression:

$$\zeta = \frac{D_c}{D}, \tag{23}$$

where D is a fractal dimension of the percolation cluster and D_c is fractal dimension of the Cantor set constructed on the surface of the percolation cluster.

Within this approach it becomes possible to explain the variation of exponent ζ with changing fraction of occupied sites in the vicinity of percolation threshold, which was revealed in numerical experiments. Increasing p results in the growth of the number of sites on the surface of a percolation cluster, through which a finite cluster can join the latter, and consequently leads to an increase of the fractal dimension of the Cantor set constructed on the considered cluster surface.

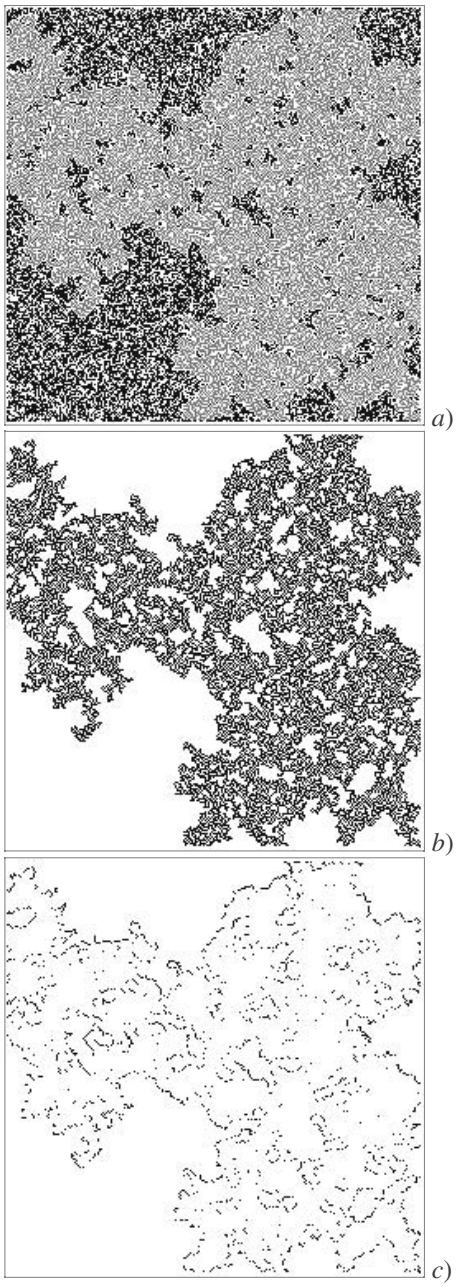

FIG. 3. Example of fractal Cantor dust constructed on the percolation cluster (square lattice 251×251, $p = 0.593$). In part (a), the finite clusters are painted in black color, sites belonging to the surface of percolation cluster are painted in dark gray, internal sites of the percolation cluster are painted in light gray; in part (b) only the sites belonging to the surface of percolation cluster are shown; in part (c) the sites belonging to the considered Cantor set are shown.

As fractal dimension D of the whole percolation cluster remains constant, then, according to Eq. (23), exponent ζ should also increase.

IV. NUMERICAL EXPERIMENT FOR DETERMINATION OF FRACTAL DIMENSION OF CANTOR DUST ON PERCOLATION CLUSTER

The obtained theoretical predictions about the relation between exponent ζ and fractal dimension of the Cantor set

TABLE I. Exponent ζ obtained for a square lattice using different methods: (1) direct calculation of the cluster size distribution, (2) on the basis of calculation of the fractal dimension of Cantor set, (3) numerical experiments for density of external surface of a percolation cluster in two dimensions [14], (4) from the traditional drop model.

p	1	2	3	4
0.59374621 ($p-p_c=0.001$)	0.37(6)±0.02	0.38(5)±0.01	0.40	0.5
0.60	0.40(8)±0.02	0.40(3)±0.01	0.40	0.5
0.61	0.43(3)±0.02	0.42(2)±0.01	0.40	0.5

constructed on the percolation cluster require additional verification. For this purpose, numerical simulation was performed. First of all, on the basis of the cluster size distribution for square lattice, the mean size of finite clusters [$\langle s\rangle = \Sigma_s s n_s(p)/\Sigma_s n_s(p)$] was calculated in region $p-p_c \approx 0.001-0.01$. This size is equal to $\langle s\rangle \approx 10$. This mean size of clusters was chosen as a basis for calculations of fractal dimension of Cantor set.

For these calculations, a special computer program was developed. The algorithm of calculations consists in four stages: (i) at a given fraction of occupied sites p, random distribution of occupied and empty sites is generated on the square lattice, (ii) in the obtained system, a percolation cluster is found and labeled [Fig. 3(a)], (iii) surface sites of the percolation cluster are found and labeled [Fig. 3(b)], and (iv) among this surface sites, such sites are found through which a finite cluster of a given size $\langle s\rangle$ can be joined to the percolation cluster [Fig. 3(c)].

At the fourth stage, calculations were performed in the following sequence. At first, a cluster containing $\langle s\rangle$ sites with an arbitrary configuration was generated. Further, all sites belonging to the surface of the percolation cluster were considered. Each site of the finite cluster was sequentially placed into all the empty sites adjacent to the surface of PC. Rotations of the finite cluster about all its sites by angels 90°, 180°, and 270° were also performed. The site of the PC surface was considered as belonging to Cantor set if there was at least one configuration which allowed to put the finite cluster in any empty site adjacent to the considered PC surface site without mutual overlapping. This set is actually the fractal Cantor dust and its fractal dimension should appear in relationships (16) and (23).

The dependence of the density of sites belonging to this set on the size of area was plotted using the log-log scale. The fractal dimension of the set is calculated from the slope of this plot [22]. This fractal dimension does not depend on the size of a system. Therefore, all calculations were performed for the fixed system size equal to $L=501$. For each considered fraction of occupied sites, 1000 samples were generated and all the characteristics was averaged over these samples. As expected, the fractal dimension of considered Cantor dust is less than 1. The results of calculation of this dimension are the following: $D_c=0.73\pm0.01$ for $p=0.59374621$, $D_c=0.76(5)\pm0.01$ for $p=0.60$, $D_c=0.80\pm0.01$ for $p=0.61$. The value of exponent ζ was calculated according to Eq. (23) with $D=91/48\approx1.895$ [13,22]. Comparison of values of exponent ζ obtained via different methods is presented in Table I. As can be seen, the proposed fractal model gives a much better agreement with the outcome of direct numerical simulations as compared with the traditional drop model.

V. CONCLUSION

In this paper, the behavior of finite clusters close to the percolation threshold has been considered on the basis of the earlier proposed kinetic approach [17]. To describe the structure of both finite clusters and the percolation cluster, the fractal model was applied. The proposed approach allowed us to establish the relation between the characteristics of cluster size distribution (exponent ζ) and nontrivial fractal properties of the percolation cluster. In particular, in the framework of the fractal model the correct value of exponent ζ was obtained and the dependence of this exponent on the fraction of occupied sites p was explained. We believe that further development of this approach will result in a better understanding of structural features of percolating systems and show a way to solving a number of urgent problems in the percolation theory.

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