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СРАВНЕНИЕ ОДНОПАРАМЕТРИЧЕСКОГО РАСПРЕДЕЛЕНИЯ ЧАСТИЦ ПО КЛАСТЕРАМ С ЛОГАРИФМИЧЕСКИ НОРМАЛЬНЫМ РАСПРЕДЕЛЕНИЕМ

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COMPARISON OF THE ONE PARAMETER DISTRIBUTION OF PARTICLES OVER CLUSTERS WITH A LOG-NORMAL DISTRIBUTION

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The analysis is given for some properties of the universal distribution of clusters over the numbers of comprising particles introduced recently in [1,2]. It has been shown that this distribution can be reduced to log-normal distribution which describes satisfactory the behaviour of the cluster distribution function especially for clusters with relatively small number of particles.

A one parameter cluster size distribution in a system of randomly spaced particles has recently been introduced in [1,2]. It is assumed that two particles belong to the same cluster, if the distance between them does not exceed a certain “radius of interaction" R. The system, therefore, is a collection of identical spheres, some of which intersect with each other, forming clusters. The question states as follows: what is the probability that a cluster contains exactly N particles. It is shown in [1,2] that the distribution of particles over clusters is determined by some universal curve independent on number of particles in the system as well as on boundary conditions and is determined by only one parameter $a = R/l_0$, where l_0 =0.554$\rho^{-1/3}$, is a most probable average distance between particles. The parameter a is called “the interaction parameter”, which plays the role of the order parameter for the system. In what follows we demonstrate the link between the universal cluster distribution and a well-known log-normal distribution. In this model, we assume that particles can move closer to any distance without affecting each other. Intersecting spheres form the “bound states". Then, as it was shown in [1,2], the distribution of particles over clusters will be determined by only one parameter a. We do not address the problems of percolation [3, 4], which are closely linked to the problem of cluster formation. Percolation assumes the existence of some boundary conditions. We study the distribution of particles over clusters independently on their shape in the infinite medium rather than the distribution of connected clusters in a random graph.

Let us renumber the clusters in decreasing order of the number of particles of which they are composed. We define the number of particles in the cluster with number k as N_k. The numbers k are sequence numbers of clusters arranged in a certain order and may be called as “ranked numbers” of clusters. By definition, $k = 1$ is a sequence number of the largest cluster containing the maximum number of particles. Surely $\sum_{k=1}^{N_0} N_k = N_0$, where N_0 is the total number of particles in the system. If we introduce a new variable $x = k/N_0$ and consider a new function of the continuous variable $N(x)$ instead of the discrete function N_k, we obtain for fixed a a universal distribution independent of the boundary conditions and on N_0. So, $N(x)$ represents the mean number of particles in a cluster with a ranked number $k = N_0 x$. Strictly speaking such universal function appears in the limit of $N_0 \to \infty$ for fixed value of the interaction parameter a. However, as it was pointed out in [1,2] the distribution is close to the universal one already for $N_0 \geq 500$. The variable x is called “a cluster rating". The distribution $N(x)$ is normalised to unity $\int_0^1 N(x)dx = 1$, where the upper limit of integration can be extended to infinity. As we see, in contrast with conventional descriptions based on the distribution of clusters over their sizes we study the distribution of particles among the clusters that consist of them.

The universal distribution function $N(x)$ for different relatively small values of interaction parameter a is shown in Fig.1. The calculations have been done by means of the Monte-Carlo simulation for $N_0 = 10^4$. Each point on the curves is the result of averaging over 50 runs. The area under these curves defines the fraction of particles ΔN that are contained in clusters with a rating in the interval $(x, x + \Delta x)$. As the parameter a increases, the distribution function $N(x)$ shifts to the left, so that $N(x) \to \delta(x)$ if $a \to \infty$; $\delta(x)$ is the Dirac's δ-function. Fig.2 demonstrates the universal distribution for larger number of a.

Curves on Figs. 1 and 2 should be interpreted as follows. The fraction of particles in clusters with rating parameter $x \in [0, 10^{-3}]$ is equal to the integral over x within this interval, which is, for $a = 2$ (curve 1, Fig.1), equal to about 0.22. This number shows the fraction of particles in any volume which are contained in clusters from this rating parameter interval Δx. These are biggest clusters in the system since they have smallest (closer to zero) values of x. I.e., for example, if the volume under consideration contains 10^6 particles, then 22% of them are contained in 1000 biggest clusters with an average number of particles in a single cluster 220. The interval $x \in [10^{-3}, 2 \times 10^{-3}]$ in this example corresponds to the fraction of particles in the same volume about 0.13. It means that another 1000 clusters contain 1.3× 10^5 particles, such that the average number of particles in one cluster is 130.

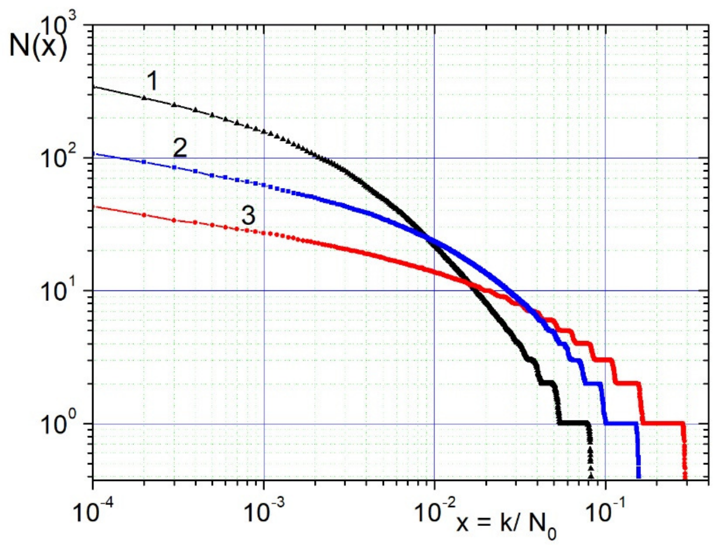

Fig.1 - Universal distribution functions $N(x)$ for different values of the interaction parameter a: $a = 2$ (curve 1), $a = 1.75$ (curve 2) and $a = 1.5$ (curve 3)

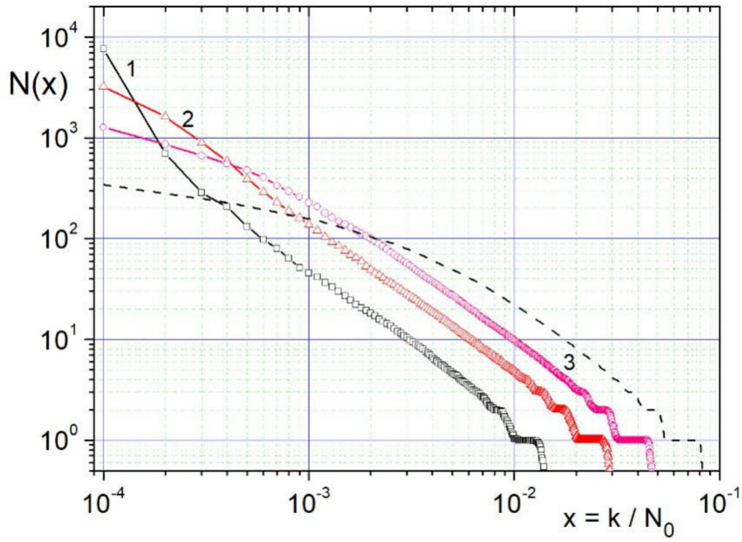

Fig.2 - The same as Fig.1 but for: $a = 3$ (curve 1, squares), $a = 2.5$ (curve 2, triangles), $a = 2.25$ (curve 3, circles) and $a = 2$ (dashed line)

For $a = 3$ (curve 1, Fig.2) the interval $x \in [0, 10^{-3}]$ contains 93% of particles in the volume considered (the area under this curve is 0.93). For the volume with $N_0 = 10^8$ particles this interval corresponds to 10^5 clusters, whereas the interval $x \in [0, 10^{-4}]$ corresponds to 10^4 clusters which contain 76% of particles, i.e. each cluster consists of 7600 particles in average. The stepped-like nature of the curves in Figs. 1 and 2 at relatively large x reflects the discrete nature of the number of particles in clusters with 1, 2, 3 ... particles.

Compare the universal distribution $N(x)$ with generally used distribution $W(x)dx$ giving the probability that the cluster contains the number of particles in the interval $(N, N + dN)$, where the number of particles N is considered as a continuous variable. To link these distributions we find a inverse function $x(N)$ from $N(x)$. Then the connection between two distribution functions is [2]

$$W(x) = \left|\frac{dx(N)}{dN}\right|, \qquad (1)$$

where the function $W(x)$ is normalized to unity for $0 < N < \infty$. We, however, take a discrete version of Eq. (1) which for $N_k \equiv N(k)$ has the form [2]

$$W(N) = k(N) - k(N + 1), \qquad (2)$$

where k is a cluster range number. The discrete function $W(N)$ is not normalized to unity and satisfies the relations [2]

$$\sum_{N=1}^{\infty} NW(N) = N_0, \qquad \sum_{N=1}^{\infty} W(N) = k_0, \qquad (3)$$

where k_0 is the maximum cluster number for which $N_k \neq 0$. While summing up Eqs. (3) one should keep in mind that $W(N) = 0$ for $N > N_{max}$, where N_{max} is number of particles in the largest cluster (i.e. for cluster with $k = 1$).

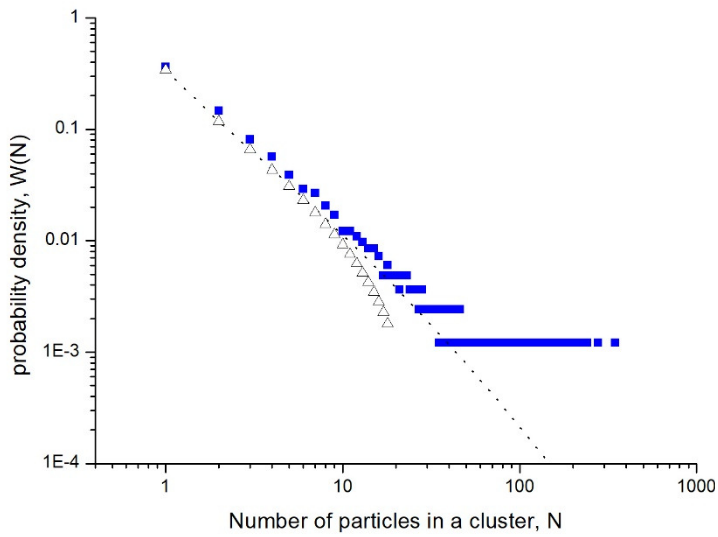

Fig.3 - The distribution function of clusters over the number of particles $W(N)$ for $a = 2$ and $N_0 = 10^4$ (squares); dashed line is the log-normal distribution (4); the light triangles is the log-normal distribution for small values of the argument (6). In this example, the mean number of particles in a cluster is $\overline{N} = 12.1$ and $\sigma = 2.23$

Let us compare the distribution function of clusters over the number of particles contained in them $W(N)$ (2) and obtained by our computer simulation, with one parameter normalized to unity log-normal distribution

$$df(N) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2} \ln^2 N\right) \frac{dN}{N}, \tag{4}$$

for which, as is well known, the mean and mean square values of particle number are

$$\overline{N} = \exp\left(\frac{\sigma^2}{2}\right), \text{ and } \overline{N^2} = \exp(2\sigma^2) . \tag{5}$$

For small values of the argument in Eq.(4) $N \ll \exp(\sigma\sqrt{2})$ the log-normal distribution (4) becomes

$$f(N) \approx \frac{1}{\sigma N\sqrt{2\pi}} \left(1 - \frac{1}{2\sigma^2} \ln^2 N\right). \tag{6}$$

Figs. 3 and 4 illustrate the comparison of the log-normal distribution (4) with the results of the computer simulation for different values of the interaction parameter a and fixed number of particles in the system $N_0 = 10^4$. The σ parameter plays a role of fitting parameter in our calculations.

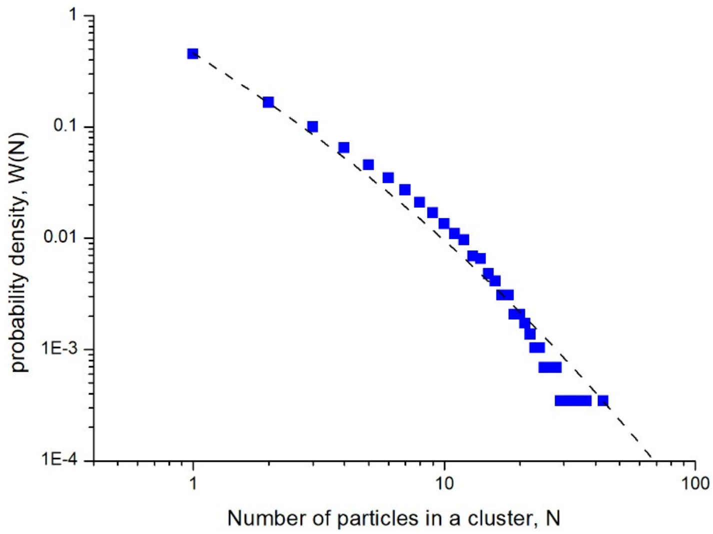

Fig.4 - The same as Fig.3 but for $a = 2$ (dark suares); solid line is the log-normal distribution (4). In this example $\overline{N}$ = 3.42 and σ= 1.57

It follows from Figs. 3 and 4 that log-normal distribution describes satisfactory the behaviour of the cluster distribution function $W(N)$ especially for clusters with relatively small number of particles. One can also learn from these figures that the cluster distribution function is very sensitive to the value of the interaction parameter a.

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