The statistics of clusters in the system of intersecting spheres randomly distributed in space

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r_0 is the interaction radius

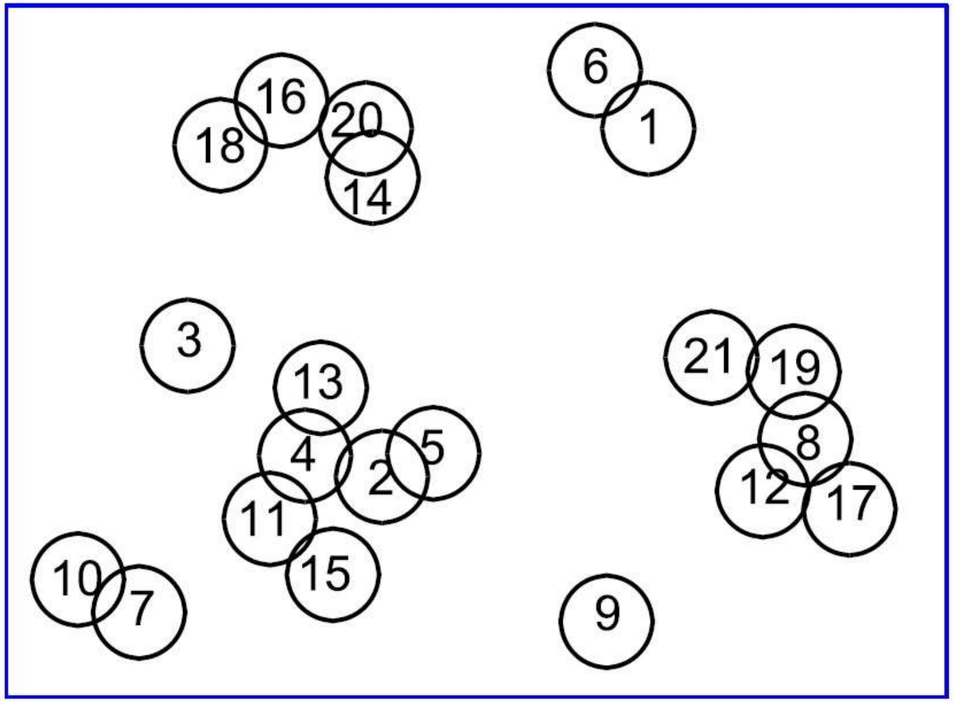
l is the most probable value of the distance between atoms

$l = 0.554 n^{-1/3}$ is the Hertz radius

$n = N / V$

$$a \equiv RATE = \frac{r_0}{l}$$

2D random system with 21 particles



$$N_1 = 6$$
$$N_2 = 5$$
$$N_3 = 4$$
$$N_4 = N_5 = 2$$
$$N_6 = N_7 = 1$$

$$N_k = \sum_{n=0}^{N} n w_k(n)$$

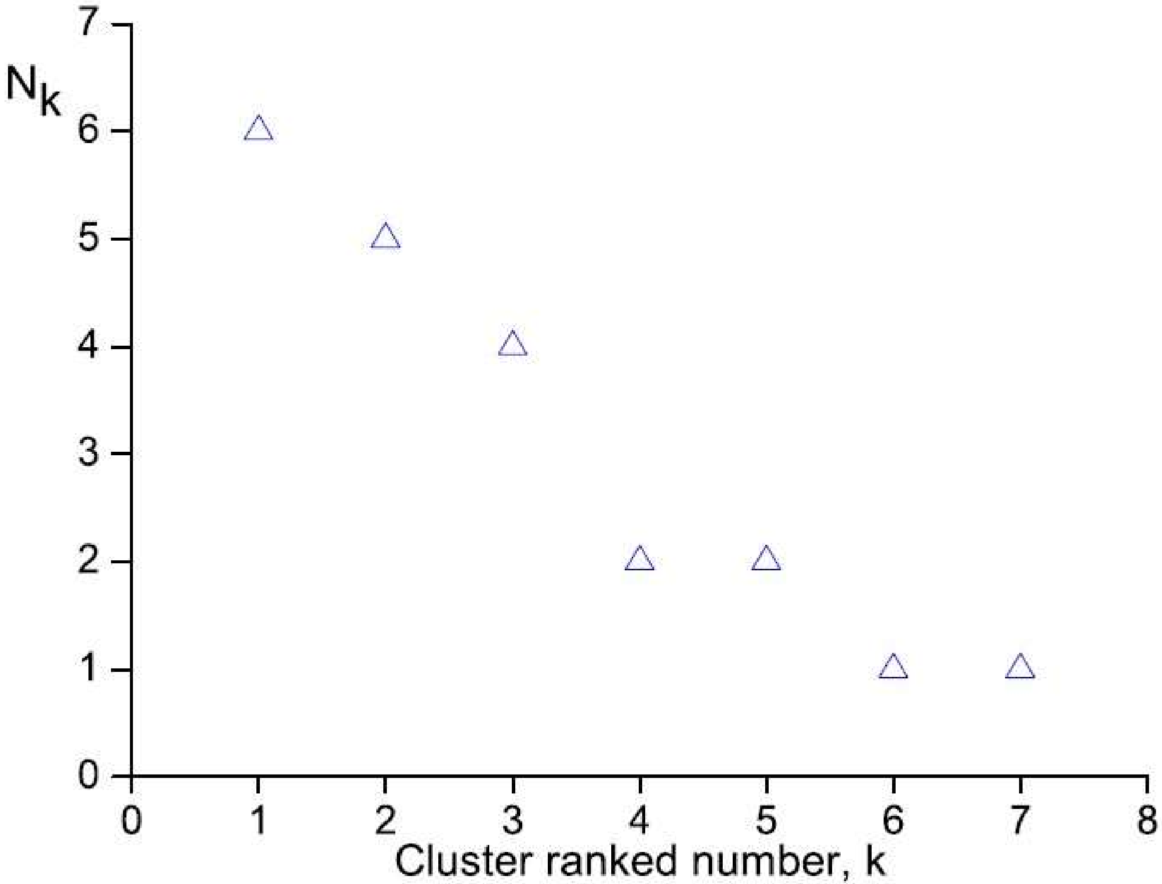
$$\sum_{k=1}^{N} N_k = N = 21$$

k *is a rank number of a cluster*

$N_k \geq N_{k+1}$ where k is a rank number of the claster

N_k is number of atoms in a cluster with a rank number k

Distribution of particles over the ranked clusters



$N_1 = 6$

$N_2 = 5$

$N_3 = 4$

$N_4 = 2$

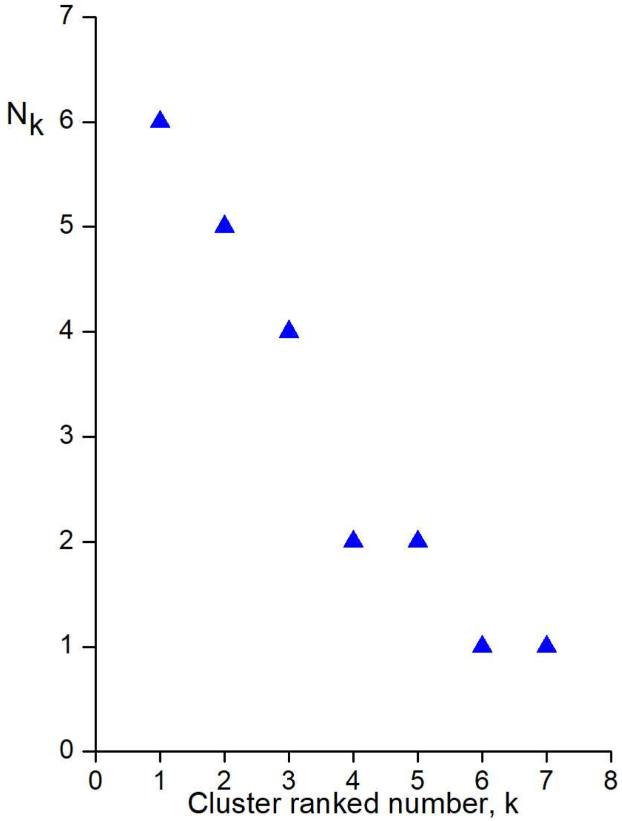
$N_5 = 2$

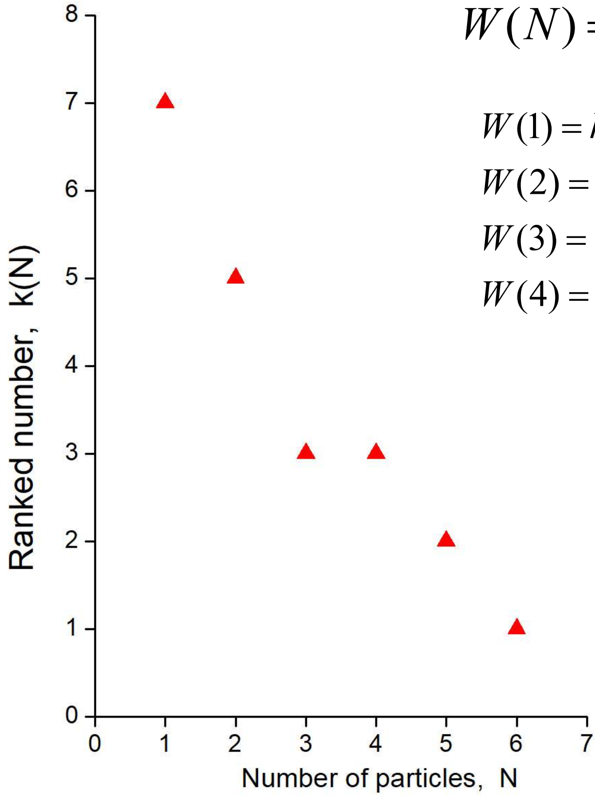
$N_6 = 1$

$N_7 = 1$

Khokonov, M.K., Khokonov, A.K. Cluster Size Distribution in a System of Randomly Spaced Particles. J Stat Phys 182, 3 (2021).

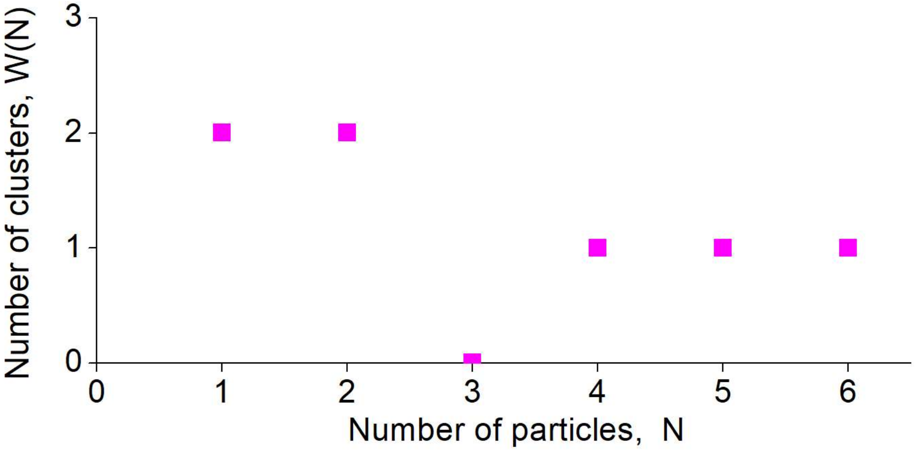
Distribution of clusters over sizes, W(N)





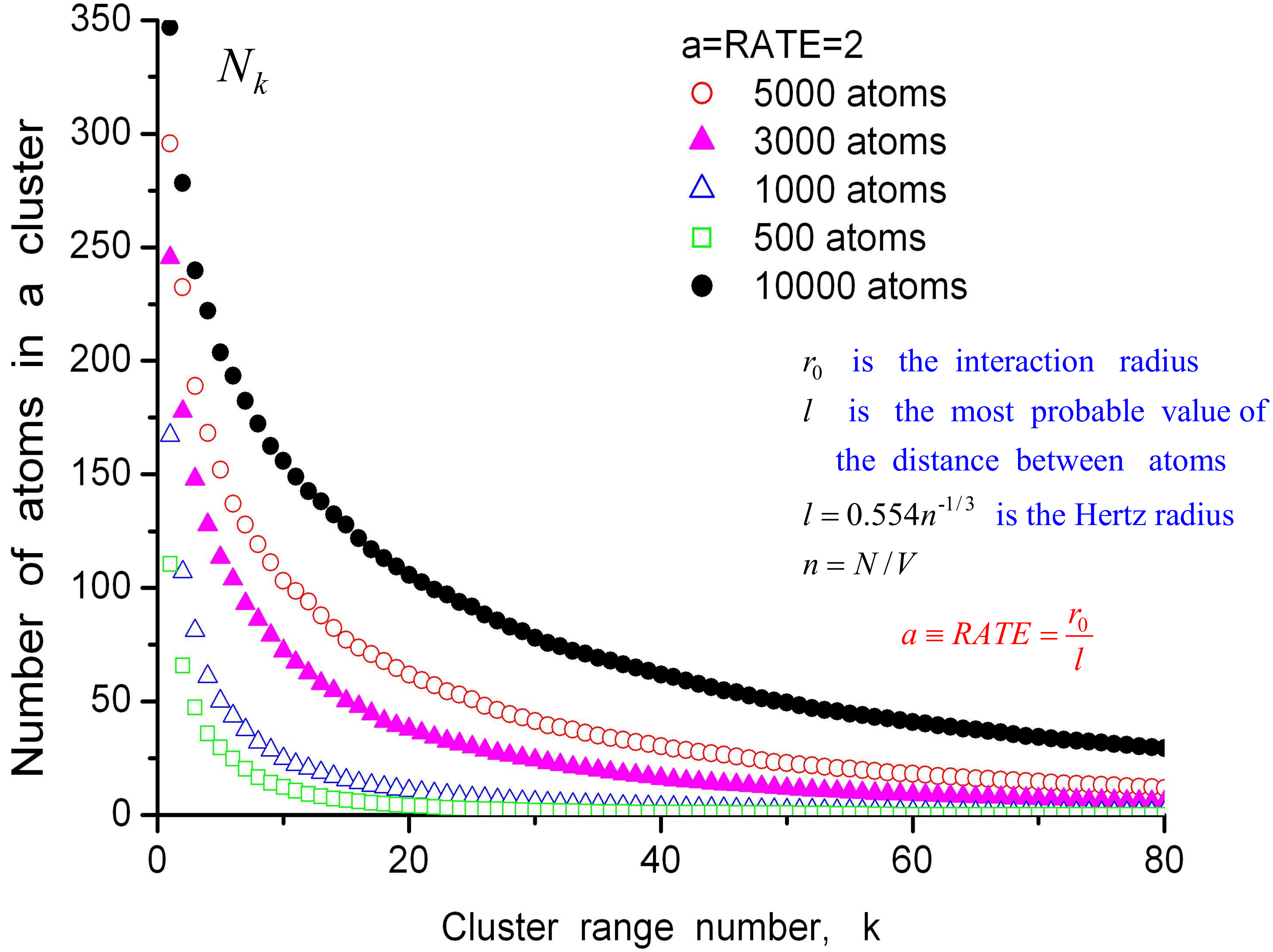
$$W(N) = k(N) - k(N+1)$$

$$W(1) = k(1) - k(2) = 7 - 5 = 2$$
$$W(2) = k(2) - k(3) = 5 - 3 = 2$$
$$W(3) = k(3) - k(4) = 3 - 3 = 0$$
$$W(4) = k(4) - k(5) = 3 - 2 = 1$$

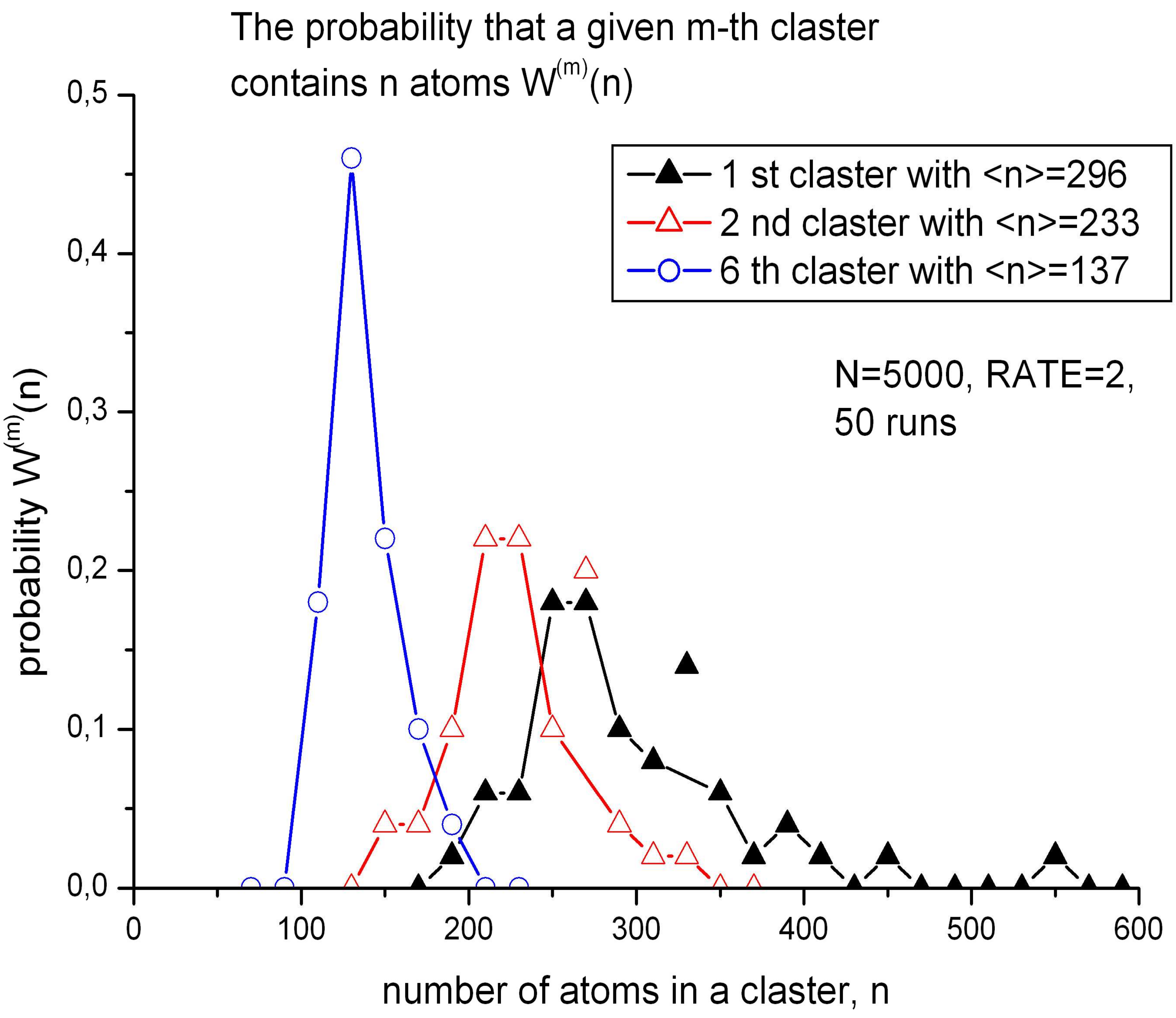


$$\sum_{N=1}^{N_{max}} N W(N) = N_0,$$

$$\sum_{N=1}^{N_{max}} W(N) = k_0.$$



350
300
250
200
150
100
50
0
20
40
60
80
N_k
Number of atoms in a cluster
Cluster range number, k
a=RATE=2
5000 atoms
3000 atoms
1000 atoms
500 atoms
10000 atoms
r_0 is the interaction radius
l is the most probable value of the distance between atoms
$l = 0.554 n^{-1/3}$ is the Hertz radius
$n = N / V$
$a \equiv RATE = \frac{r_0}{l}$



The probability that a given m-th claster
contains n atoms W(m)(n)
1 st claster with <n>=296
2 nd claster with <n>=233
6 th claster with <n>=137
N=5000, RATE=2,
50 runs
probability W(m)(n)
number of atoms in a claster, n
0,0
0,1
0,2
0,3
0,4
0,5
0
100
200
300
400
500
600

Функция распределения кластеров по размерам (числу частиц)

$W(N)-$ вероятность того, что кластер содержит ровно N частиц

$$\sum_{N=1} W(N) = 1. \qquad (1)$$

Из численной функции N_k находим обратную $k(N)$. Тогда

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

Логнормальное распределение

$$df(N) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}\ln^2 N\right)\frac{dN}{N} \qquad (3)$$

$$\int_0^\infty f(N)dN = 1 \qquad (4)$$

$$\overline{N} = \int_0^\infty Nf(N)dN = \exp\left(\frac{\sigma^2}{2}\right) \qquad (5)$$

$$\overline{N^2} = \int_0^\infty N^2 f(N)dN = \exp\left(2\sigma^2\right) \qquad (6)$$

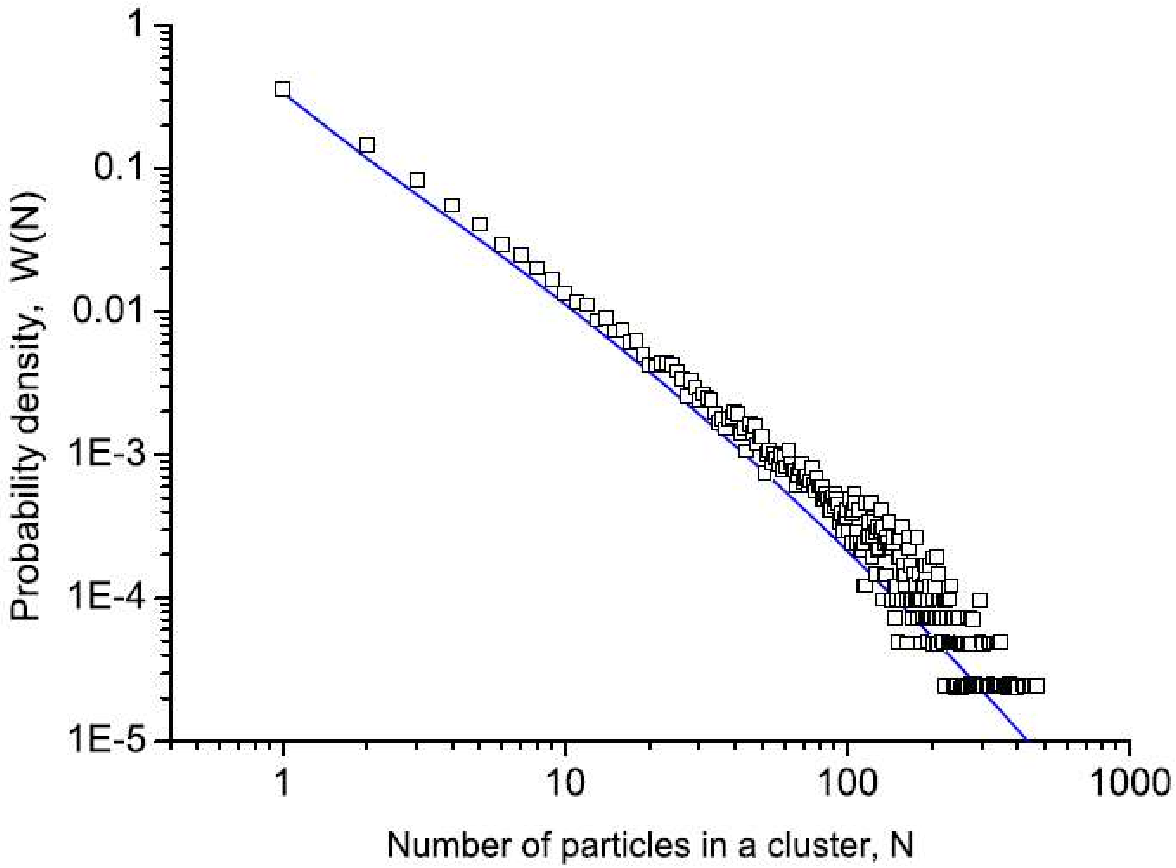


Fig. 8 The distribution function of clusters over the number of particles $W(N)$ for $a = 2$ and $N_0 = 10^4$ (squares); solid line is the log-normal distribution (8). In this example, the mean number of particles in a cluster is $\overline{N} = 12.1$ and $\sigma = 2.23$

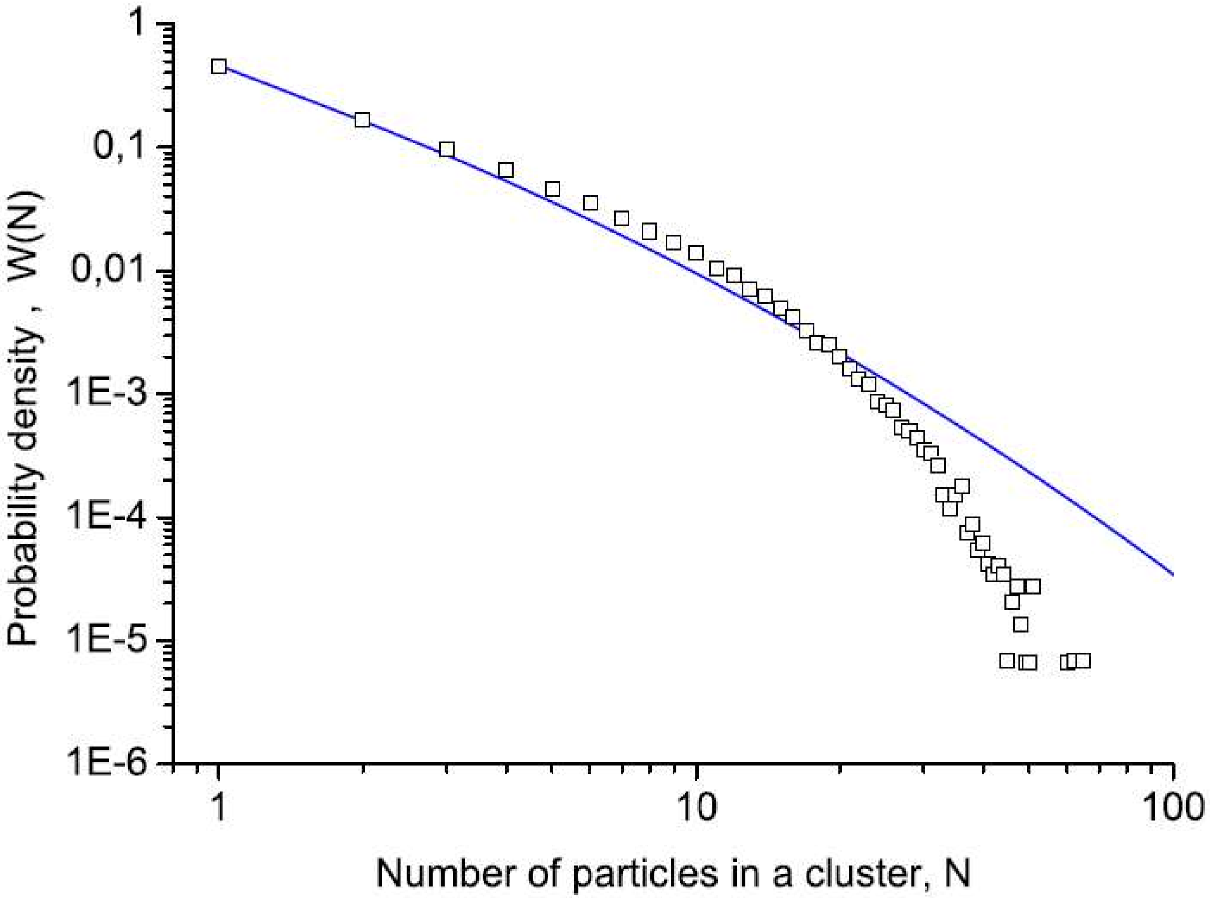
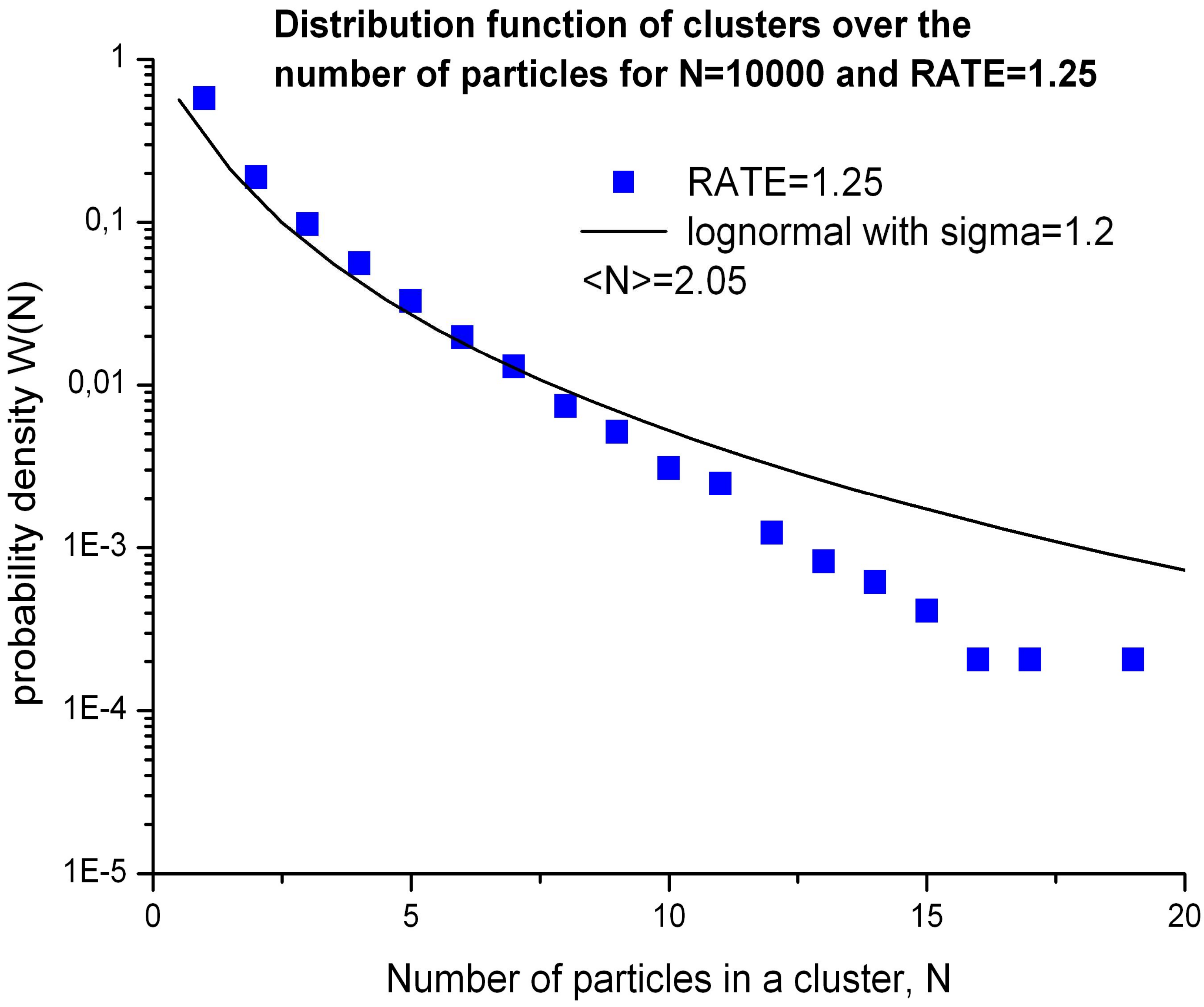
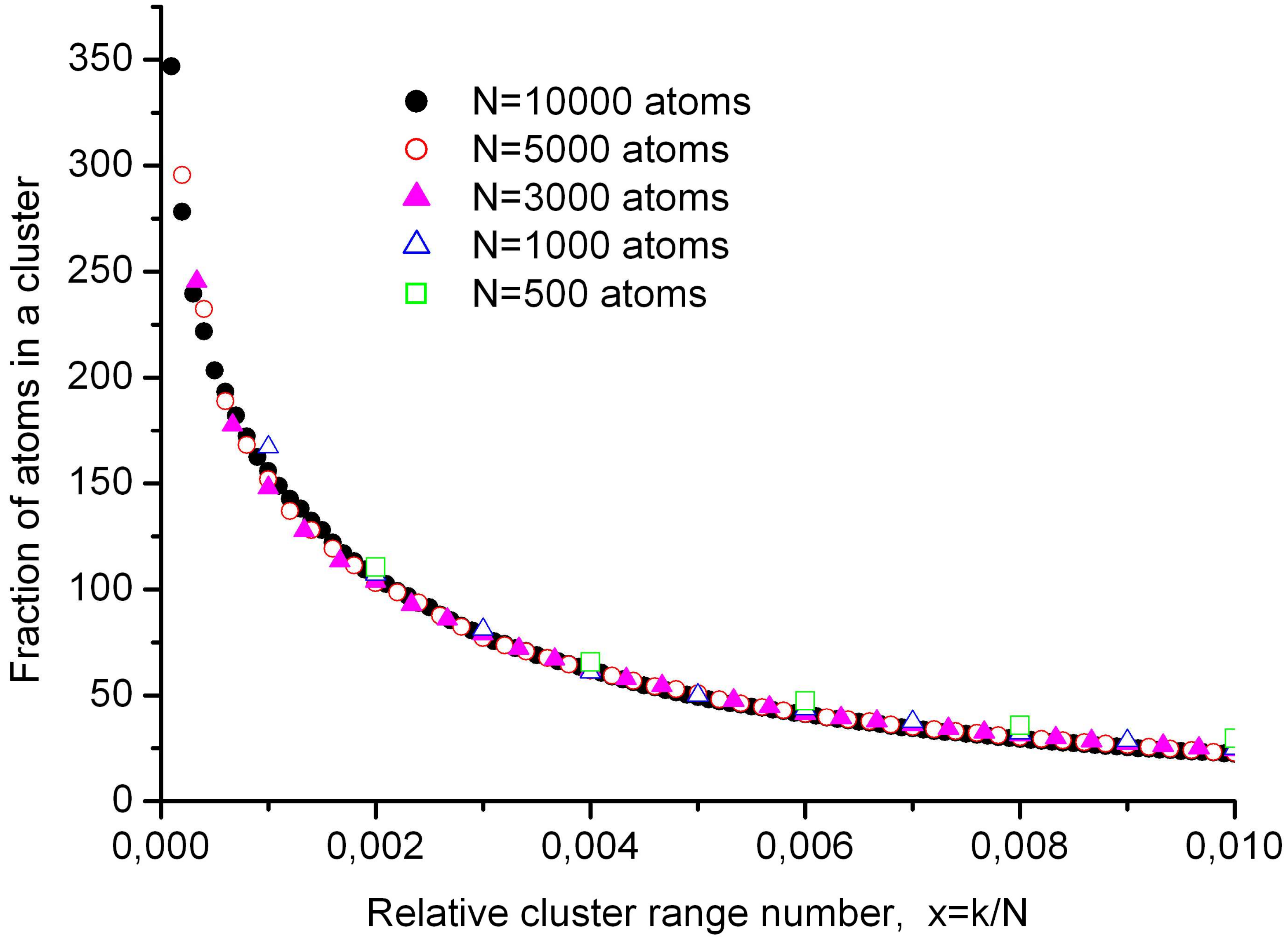


Fig. 9 The same as Fig. 8 but for $a = 1.5$. The log-normal distribution (8) is shown by the full curve. In this case $\overline{N} = 3.42$ and $\sigma = 1.57$


Distribution function of clusters over the
number of particles for N=10000 and RATE=1.25
RATE=1.25
lognormal with sigma=1.2
<N>=2.05
probability density W(N)
Number of particles in a cluster, N
1
0,1
0,01
1E-3
1E-4
1E-5
0
5
10
15
20

For relative cluster range number $x = k / N$ distribution becomes independent on N and becomes universal depending only on one parameter RATE $\equiv a = r_0/l$



Standard distribution $N(x)$

$$\int_0^1 N(x)dx = 1$$

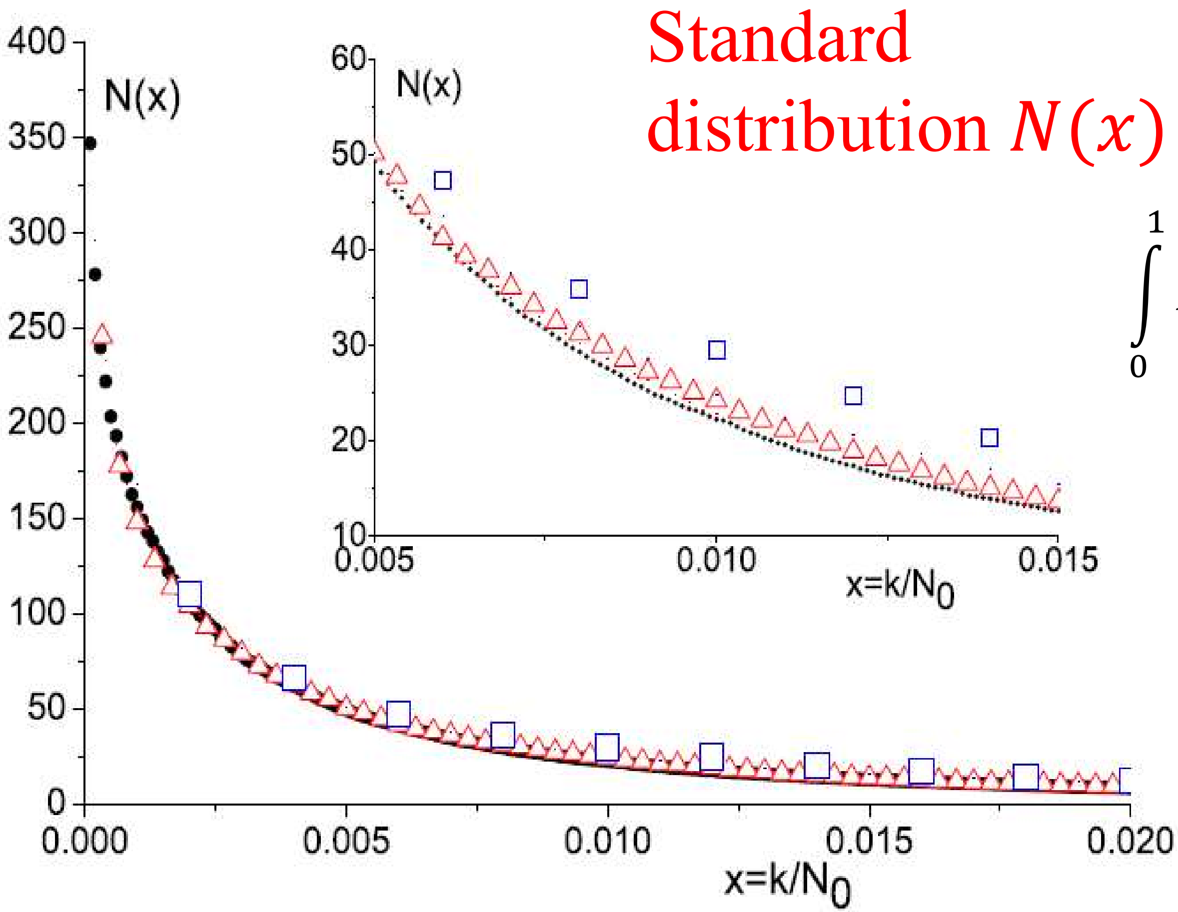


Fig. 10 The distributions of particles over the clusters $N(x)$ as a function of the continuous variable $x = k/N_0$ (the cluster rating). Distributions correspond to the data shown in Fig. 3 for $a = 2$ and different numbers of particles in the system N_0: $N_0 = 10^4$ (dots); $N_0 = 3000$ (triangles) and $N_0 = 500$ (squares). The upper plot shows the function $N(x)$ in the interval , $0.005 < x < 0.015$, on an enlarged scale

x is a relative ranked cluster number: $0< x<1$

$N(x)$ is the mean number of particles in a cluster with ranked number $k = N_0 x$

$$N(x) \rightarrow x(N)$$

$$W(N) = \left|\frac{dx(N)}{dN}\right|$$

$$0 < x < 1, \qquad 0 < N < \infty$$

$$\int_0^\infty W(N)dN = 1$$

$$N(x) = (1-\alpha)x^{-\alpha}$$

$$dW(N) = \frac{(1-\alpha)^{1/\alpha}}{\alpha} N^{-(1+\alpha)/\alpha} dN$$

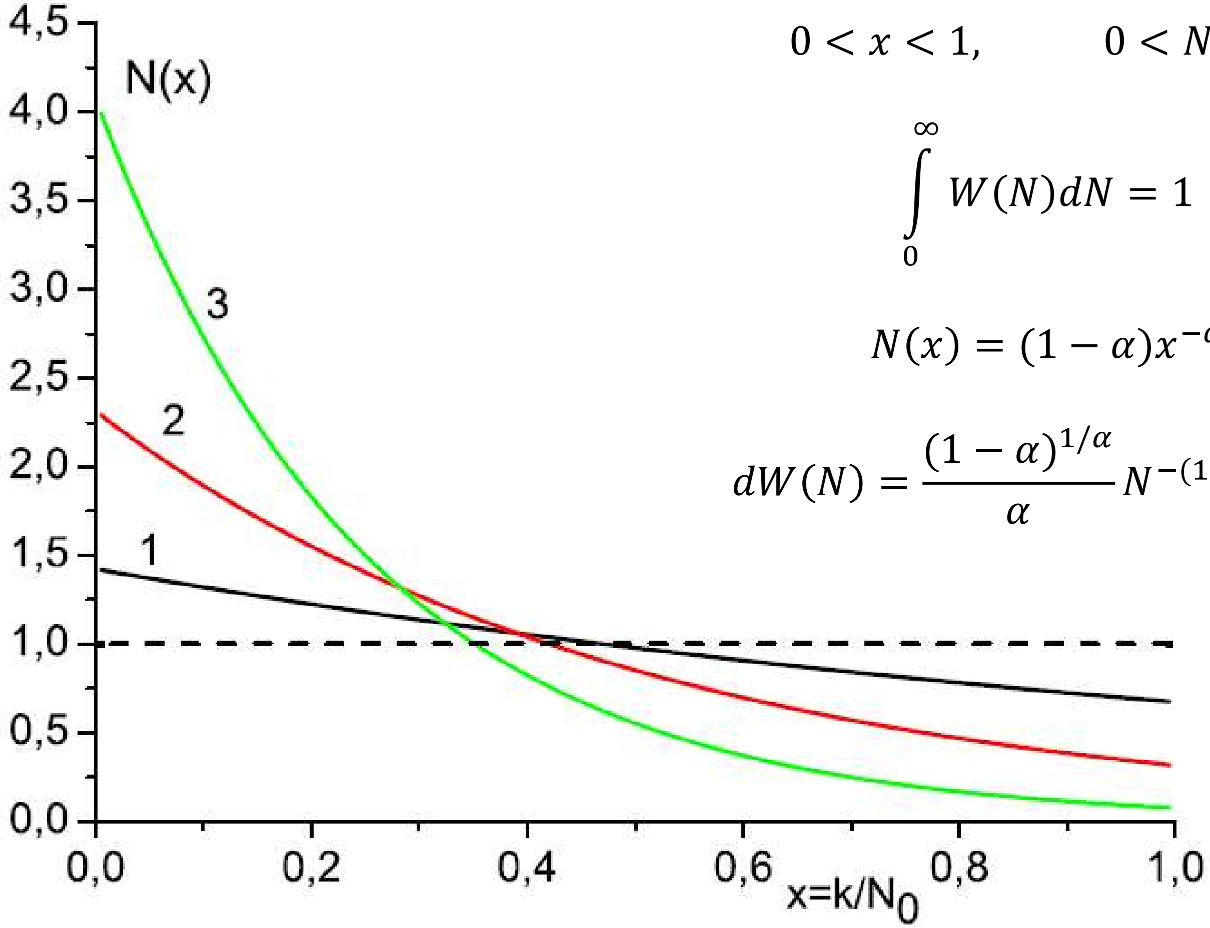


Fig. 11 Illustration of the behavior of the distribution function $N(x)$ for different values of the interaction parameter a. The dashed line refers to the system consisting of single particles only ($a = 0$). Lines 1, 2 and 3 correspond to the increase of the parameter a: $a_3 > a_2 > a_1$

Standard distribution $N(x)$

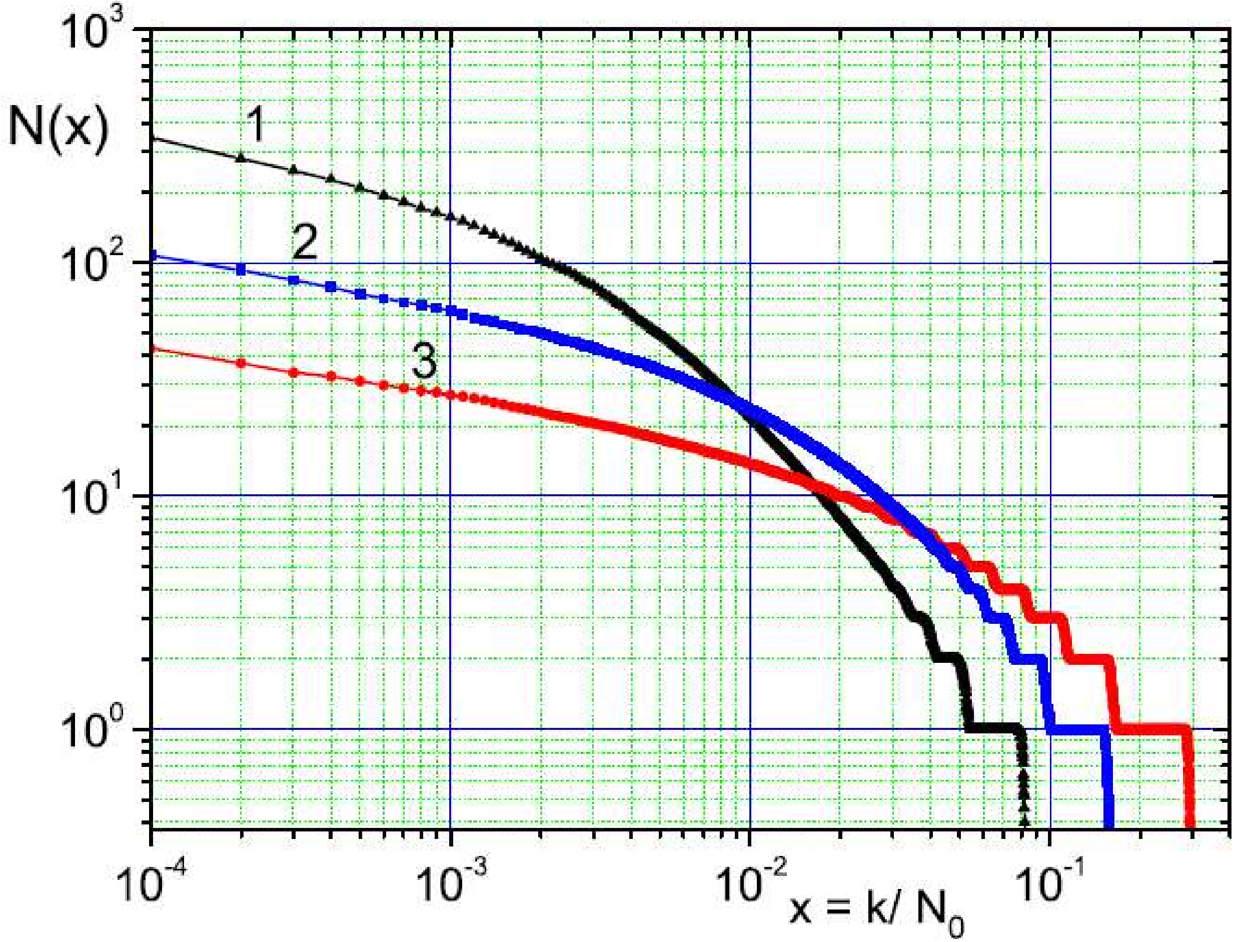


Fig. 12 Distribution functions $N(x)$ for different values of the interaction parameter a: $a = 2$ (curve 1), $a = 1.75$ (curve 2) and $a = 1.5$ (curve 3)

Standard distribution $N(x)$

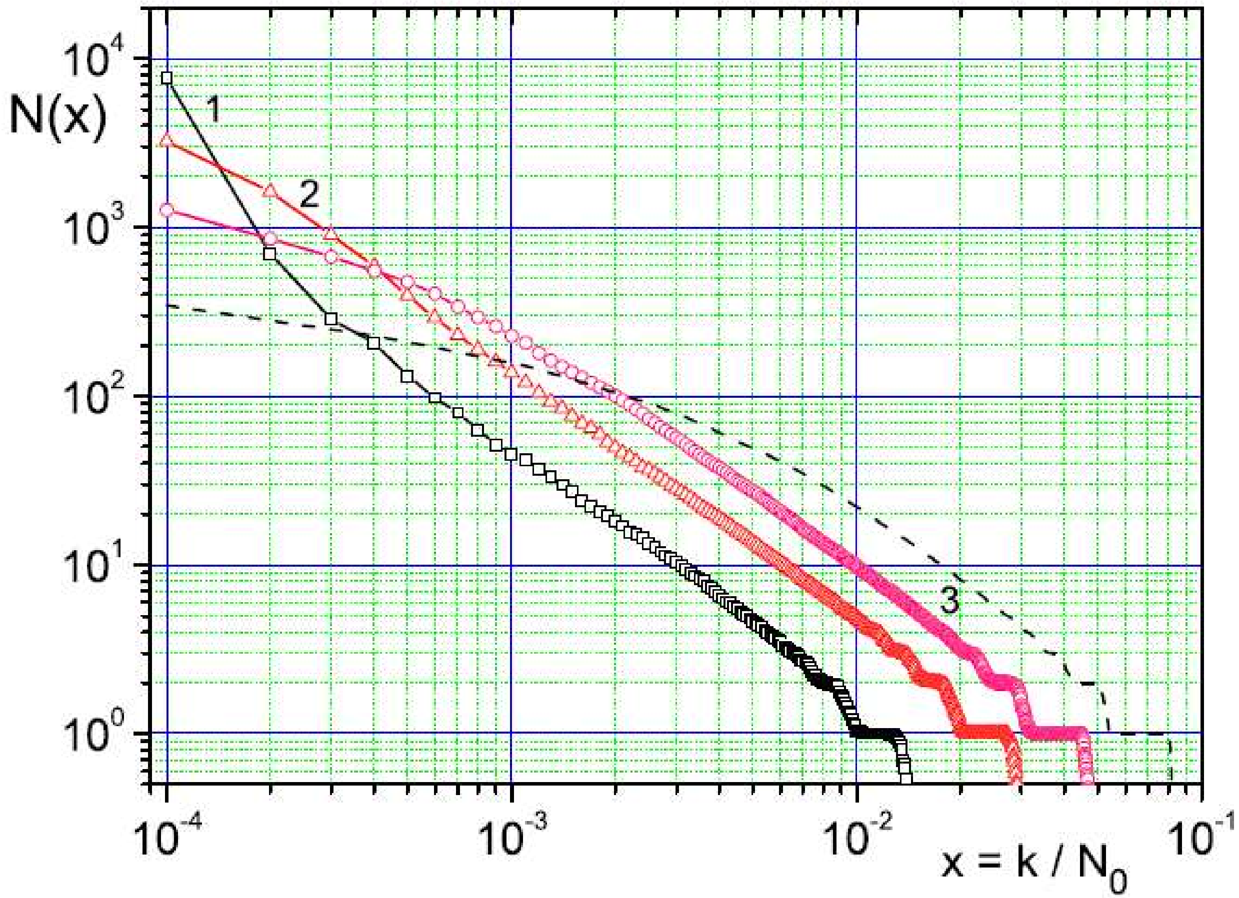


Fig. 13 The same as Fig. 12 but for: $a = 3$ (curve 1, squares), $a = 2.5$ (curve 2, triangles), $a = 2.25$ (curve 3, circles) and $a = 2$ (dashed line)

Fraction of particles in a largest cluster

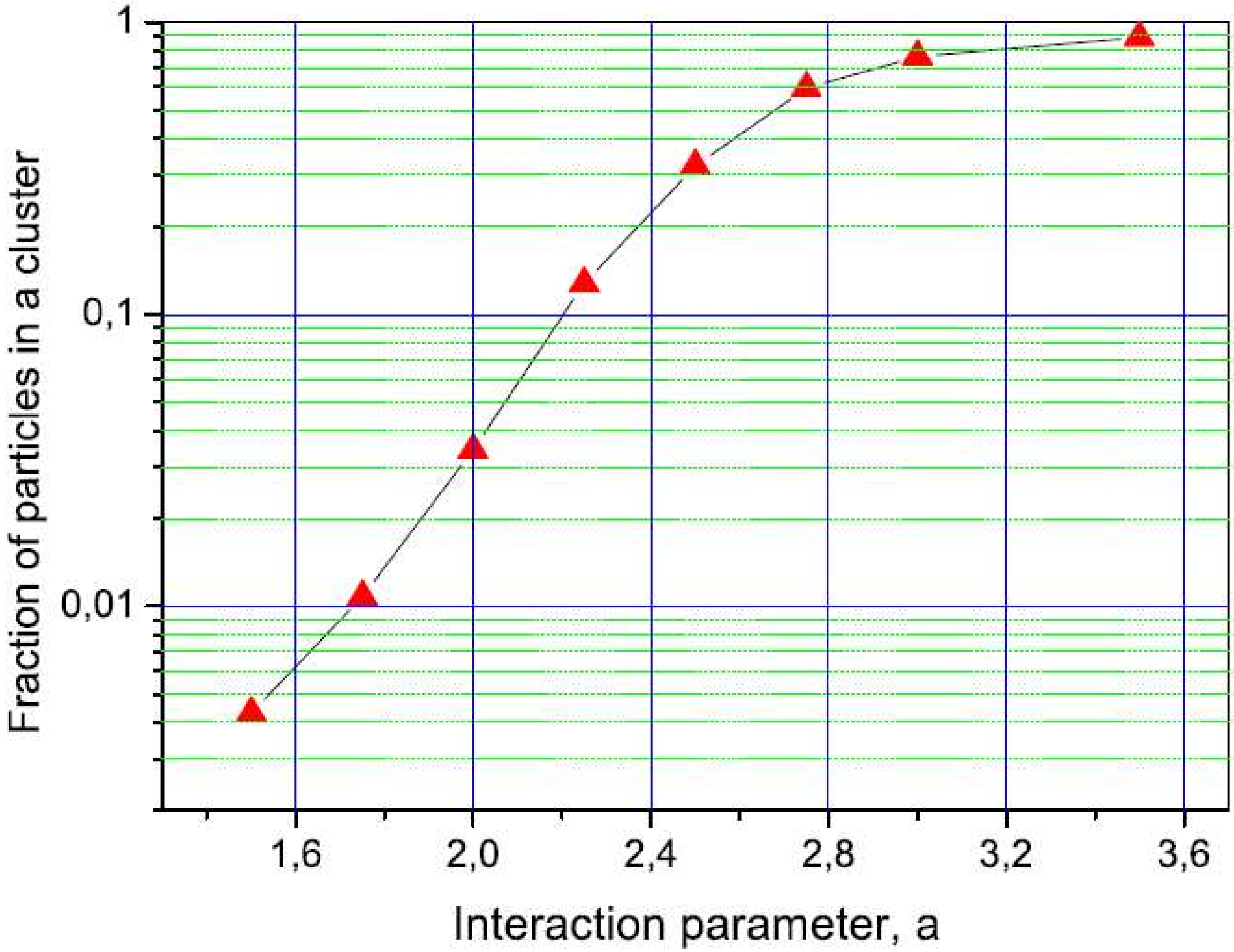
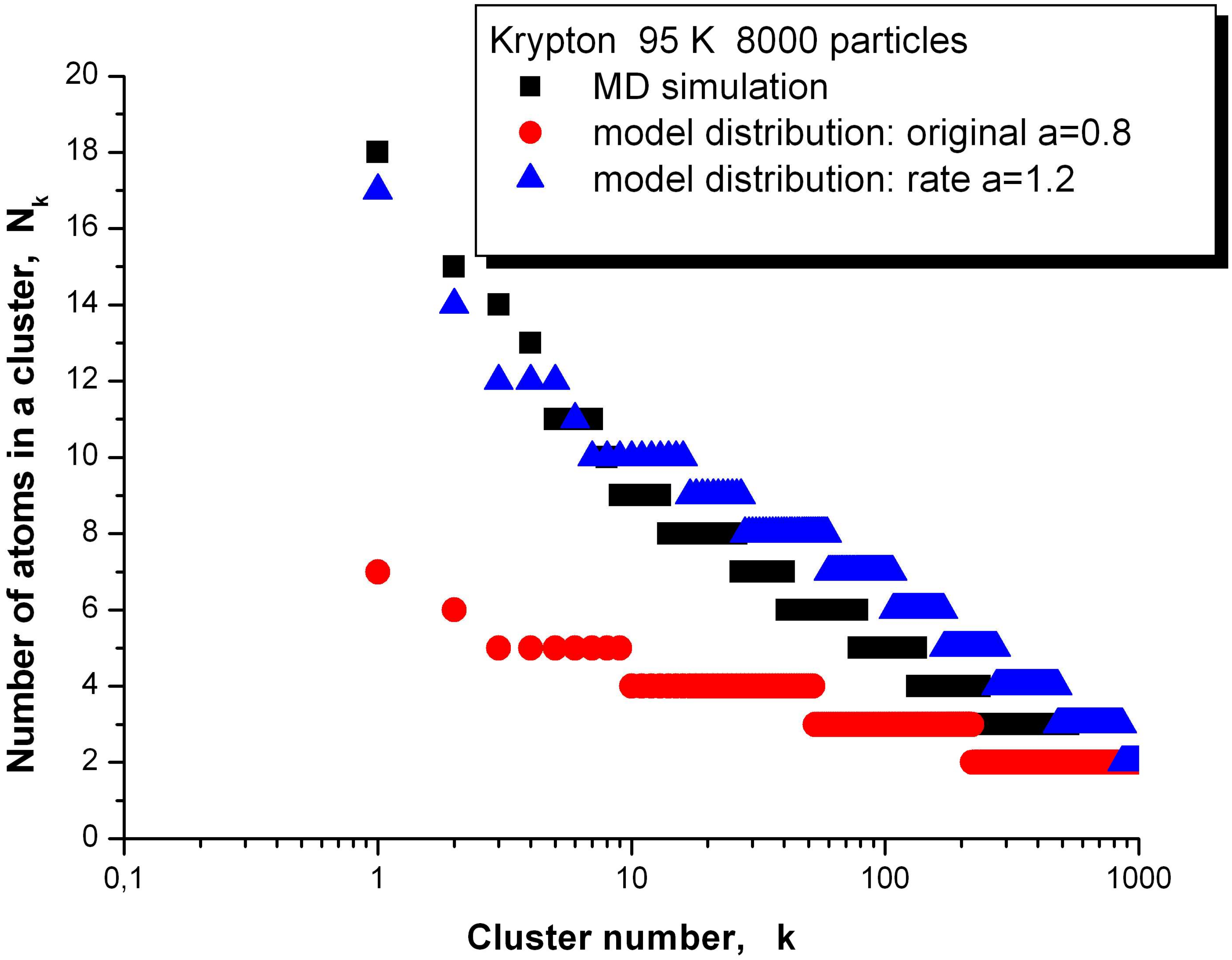
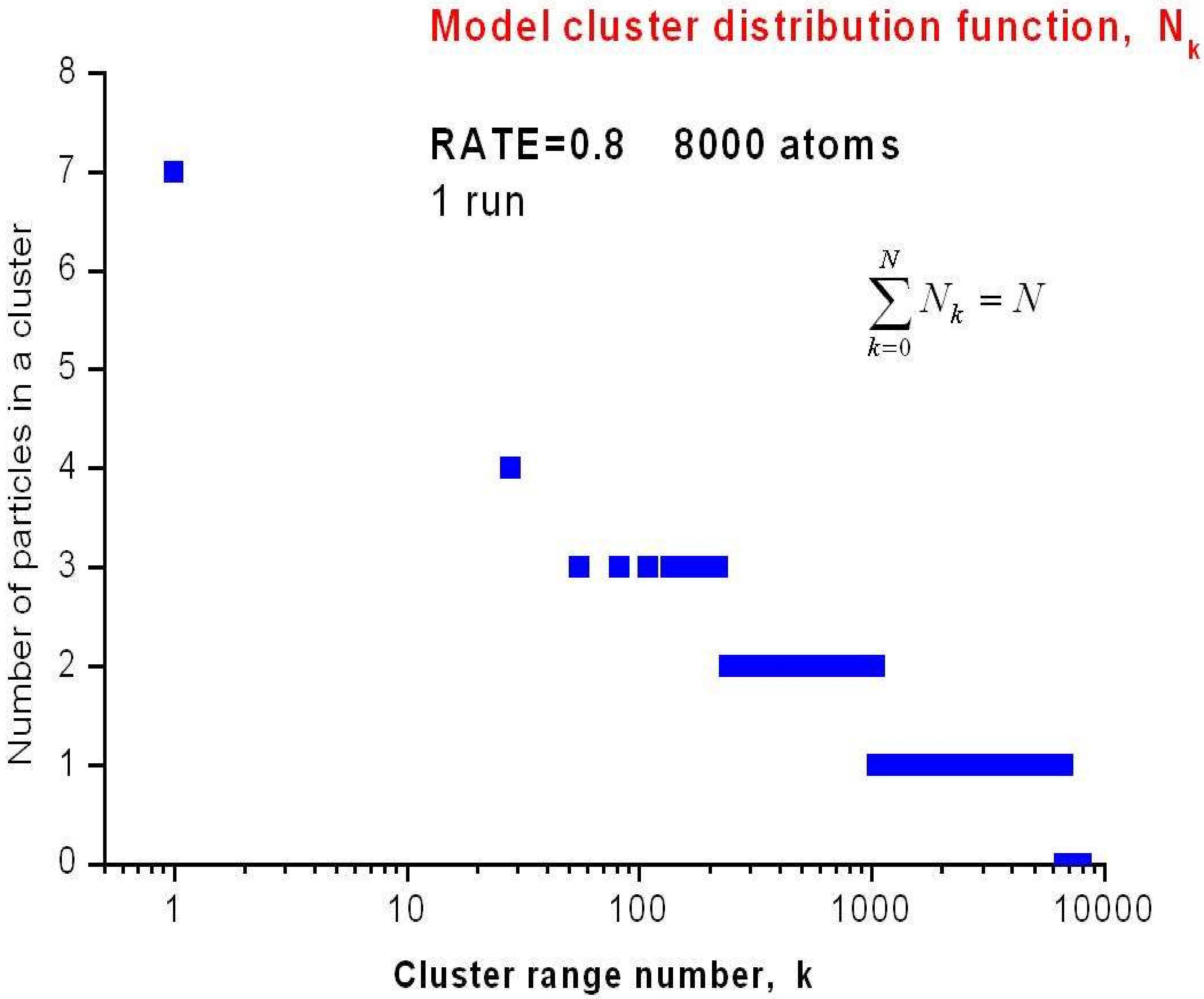
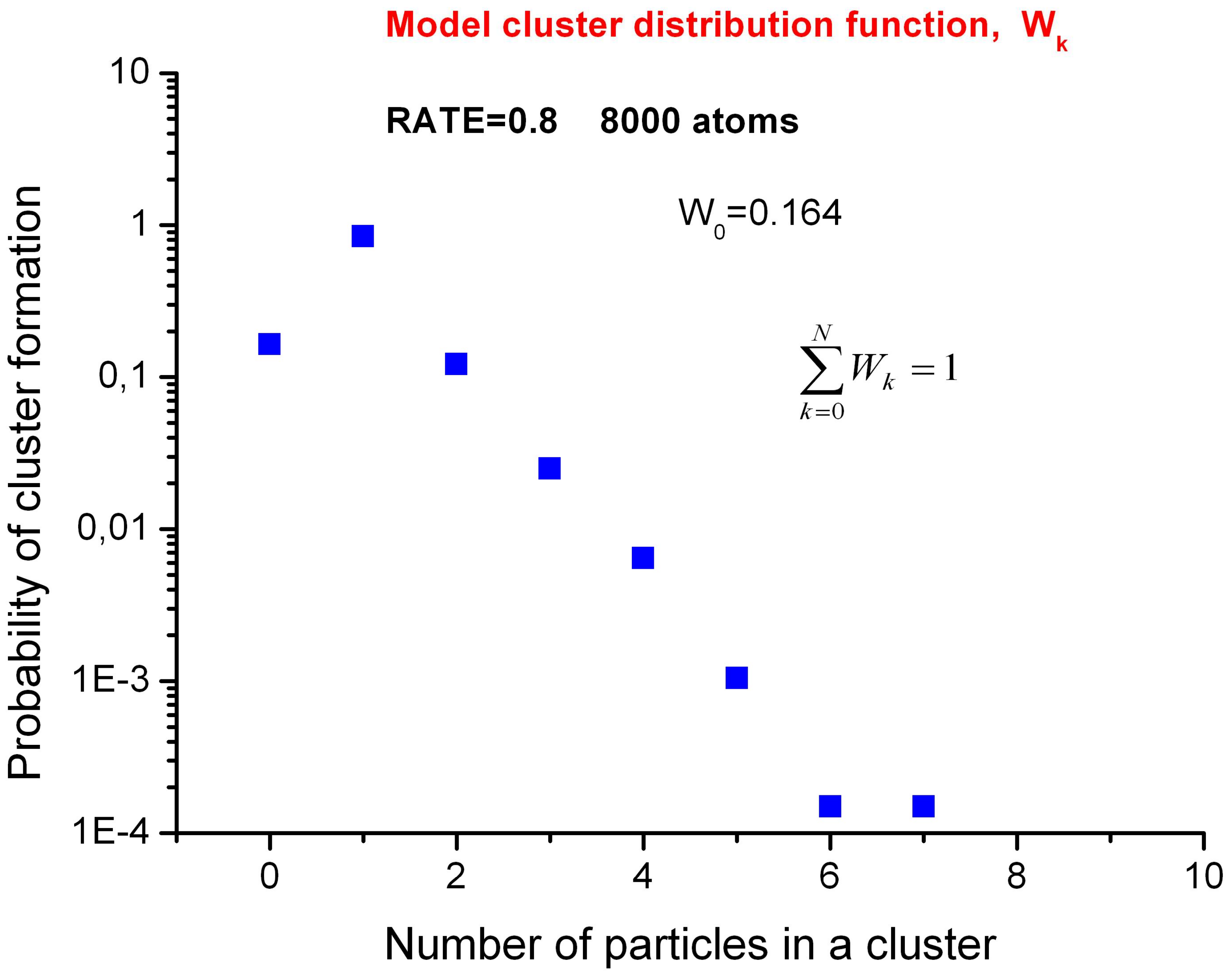


Fig. 14 The fraction of particles contained in the cluster of the largest size, depending on the interaction parameter *a*

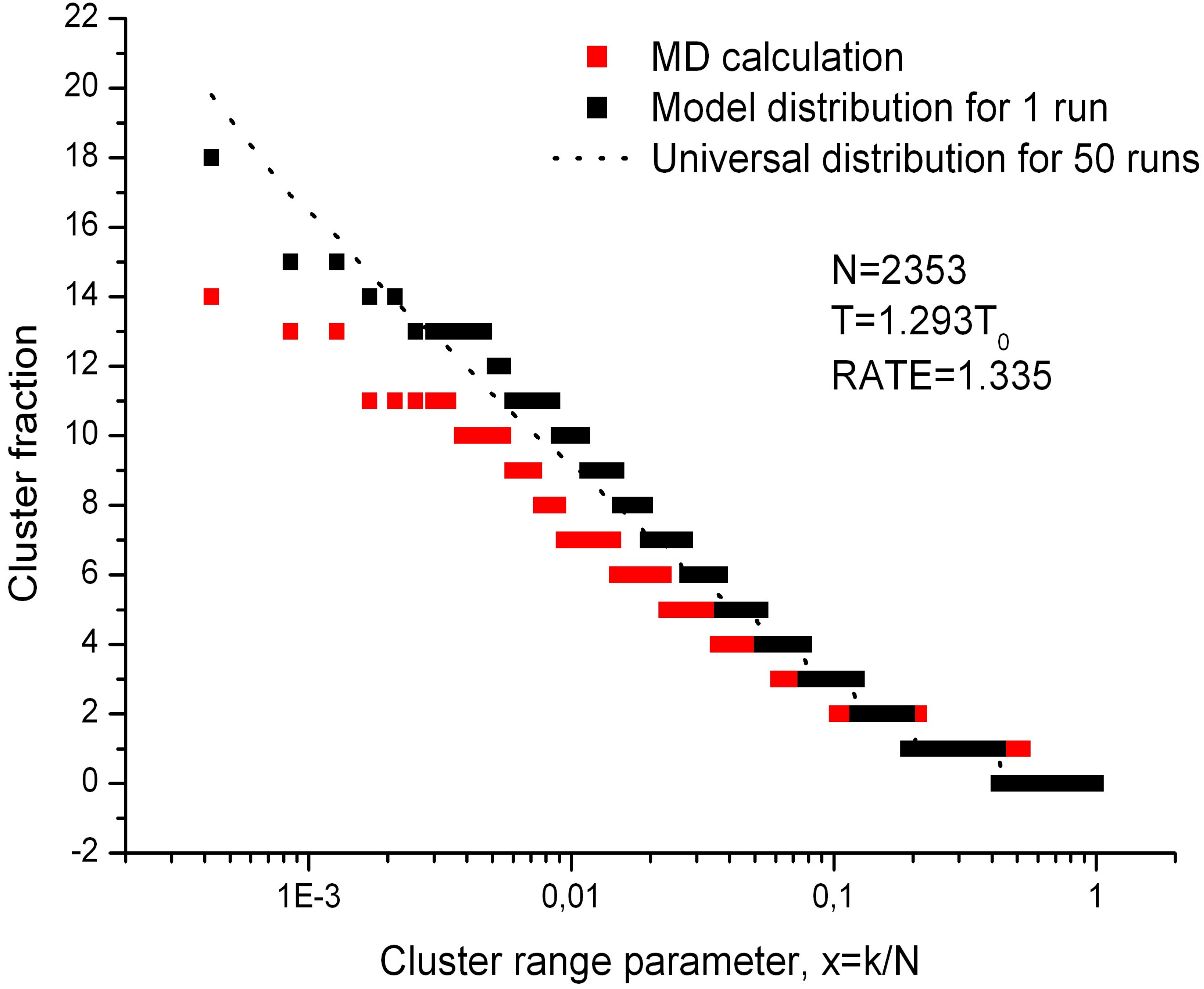


Krypton 95 K 8000 particles
MD simulation
model distribution: original a=0.8
model distribution: rate a=1.2
Number of atoms in a cluster, N_k
Cluster number, k
0
2
4
6
8
10
12
14
16
18
20
0,1
1
10
100
1000


Model cluster distribution function, N_k
RATE=0.8 8000 atoms
1 run
$$\sum_{k=0}^{N} N_k = N$$
Number of particles in a cluster
0
1
2
3
4
5
6
7
8
1
10
100
1000
10000
Cluster range number, k



Model cluster distribution function, W_k
RATE=0.8 8000 atoms
W_0=0.164
$$\sum_{k=0}^{N} W_k = 1$$
Probability of cluster formation
10
1
0,1
0,01
1E-3
1E-4
0
2
4
6
8
10
Number of particles in a cluster


MD calculation
Model distribution for 1 run
Universal distribution for 50 runs
N=2353
T=1.293T0
RATE=1.335
Cluster fraction
Cluster range parameter, x=k/N
22
20
18
16
14
12
10
8
6
4
2
0
-2
1E-3
0,01
0,1
1

25.02.2017

Conclusions

- The one parameter standard cluster distribution exists which properly reflects the realistic conditions