

Improved percolation thresholds for rods in three-dimensional boxes

R. Florian^a and Z. Néda^b

^aCenter for Cognitive and Neural Studies, str. Saturn 24, RO-3400 Cluj-Napoca, Romania

florian@coneurat.org

^bBabeş-Bolyai University, Dept. of Physics, str. Kogălniceanu 1, RO-3400 Cluj-Napoca, Romania

zneda@phys.ubbcluj.ro

(September 25, 2001)

We improve our previous results for the percolation thresholds of isotropically oriented rods in three dimensional boxes. We prove again the applicability of the excluded volume rule in the slender-rod limit (radius/length $\rightarrow 0$). Other limits for the rod sizes are discussed and important finite-size effects are revealed.

PACS numbers: 64.60.Ak, 02.50.Ng, 05.40.+j

We have previously [1] revealed errors of earlier simulations [2] for the percolation of permeable rods in three dimensions. We have also presented corrected results [3] that confirm the excluded volume theory. In this short preprint we give more accurate numerical values for the percolation thresholds, obtained by extended computer simulations. Given the importance of such results in designing composite materials (electrically conducting polymers, fiber-inforced plastics) it is useful to summarize and discuss the obtained percolation thresholds.

The studied system is formed by permeable sticks with the form of capped cylinders (cylinders of length L and radius R capped with two hemispheres of radius R). It was conjectured [4] that the percolation threshold, q_p , is proportional to the inverse of the expected excluded volume, V_{ex} :

$$q_p = \frac{N_c}{V} \propto \frac{1}{V_{ex}} \quad (1)$$

(We denoted by N_c the number of sticks at percolation and by V the volume of the cube in which the percolation problem is considered.) For sticks with the form of capped cylinders the excluded volume is given by

$$V_{ex} = \frac{32\pi}{3}R^3 + 8\pi LR^2 + 4L^2R \langle \sin(\gamma) \rangle, \quad (2)$$

where $\langle \sin(\gamma) \rangle$ is the average value of $\sin(\gamma)$ for two randomly positioned sticks, and γ is the angle between them. For isotropic orientation of rods ($\langle \sin(\gamma) \rangle = \pi/4$) it was shown by a cluster expansion method [5] that the proportionality in (1) becomes equality in the $R/L \rightarrow 0$ slender-rod limit. This equality is known as the excluded-volume rule.

We have studied the problem inside a cube with unit sizes. In order to preserve homogeneity near the cube's frontiers, the coordinates of the centers of the cylinders were generated uniformly in the interval $[-(L/2+R), 1+(L/2+R)]$. The orientation of the cylinders was isotropic. We detected the intersection of two capped cylinders by

calculating the minimum distance between points on the two axes of the corresponding cylinders and by comparing this distance with $2R$. Each time a new stick was generated, it was assigned to a cluster if it intersected a previous one, otherwise a new cluster was created; a stick may also unify two or more clusters that were previously separated. We considered percolation achieved when a cluster spanned the cube from one face to the opposite one. The critical concentration is given by the number of sticks inside the cube at percolation, N_c . If a capped cylinder was only partially inside the cube, it contributed to N_c with a fractional value less than one, corresponding to the fraction of its volume inside the cube to its total volume. We generated many percolation realizations (usually 5000) for each considered L and R pair, and the average N_c was calculated as the mean of the obtained percolation thresholds.

The obtained results are summarized in Figs. 1 - 3.

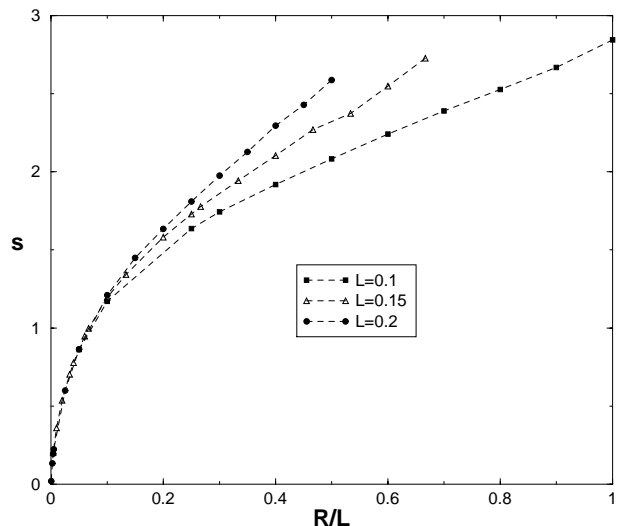


FIG. 1. $s = q_p V_{ex} - 1$ as a function of the R/L aspect ratios of the sticks. Data for three different stick lengths, L , are presented.

On Fig. 1 we plot the quantity $s = q_p V_{ex} - 1$ as a function of R/L for various fixed L values. In the limit $R/L \rightarrow 0$ our simulations suggest the analytically predicted $s = 0$ relation [5]. This is nicely proven by our large-scale simulation data for $L = 0.2$ (for systems of up to $N_c = 8 \cdot 10^4$ rods). The convergence for the applicability of the excluded volume rule is however rather poor. As an example in this sense we found in the $R/L \rightarrow 0$ limit ($R/L < 0.05$), for $L = 0.15$, s scaling as a function of R/L with an exponent of 0.58. From Fig. 1 is also clear that for smaller values of L and the same R/L ratios the value of s gets smaller. There are thus important finite-size effects, which are less evident in the $R/L \rightarrow 0$ limit.

We have checked that in the limit of $L \rightarrow 0$ the $s = 0$ equality still does not hold. This is clear from our simulation data for $R/L = 0.5$, $R/L = 0.25$ and $R/L = 0.1$. The data presented on Fig. 2 suggest that in the limit $L \rightarrow 0$, s is linearly converging to 1.58, 1.46 and 1.14 for $R/L = 0.5$, $R/L = 0.25$ and $R/L = 0.1$, respectively. This linear convergence may be useful for approximating the s value given R and L .

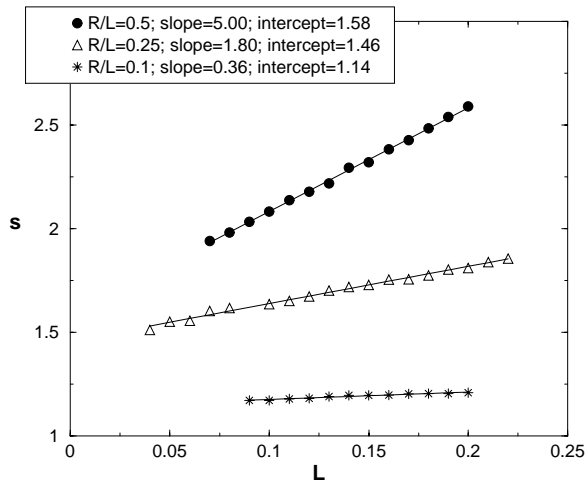


FIG. 2. Finite size effects: $s = f(L)$ for two different aspect ratios of the sticks. Continuous lines are the best linear fit. In the $L \rightarrow 0$ limit we got $s = 1.58$, $s = 1.46$ and $s = 1.14$ for $R/L = 0.5$, $R/L = 0.25$ and $R/L = 0.1$, respectively.

Problems with the applicability of the excluded-volume rule appears also in the $L \rightarrow 1$ limit, where the length of the sticks approaches the characteristic length of the box. This is nicely visible from Fig. 3 where we have plotted s as a function of R/L for two fixed R values ($R = 0.01$ and $R = 0.02$, respectively). In the limit of very small R/L values one can observe again the increasing difference from the $s = 0$ theoretical result, due to L values approaching the characteristic box size.

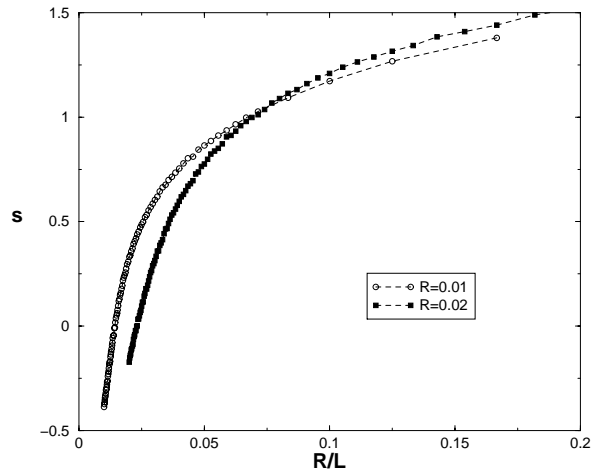


FIG. 3. $s = f(R/L)$ for two different radii of the sticks.

In conclusion, our results suggest that the excluded-volume rule is applicable in the slender-rod limit ($R/L \rightarrow 0$) for stick lengths much smaller than the characteristic box-size. For all other cases important deviations from this rule are present. Decreasing the rod length improves the applicability of the excluded-volume rule, but the $R/L \rightarrow 0$ condition is still necessary in the $L \rightarrow 0$ limit.

-
- [1] Z. Neda, R. Florian; cond-mat/9804326 (1998)
 - [2] I. Balberg, N. Binenbaum and N. Wagner; Phys. Rev. Lett. **52**, 1465 (1984)
 - [3] Z. Neda, R. Florian and Y. Brechet; Phys. Rev. E **59**, 3717 (1999)
 - [4] I. Balberg, C.H. Anderson, S. Alexander and N. Wagner; Phys. Rev. B **30**, 3933 (1984)
 - [5] A.L.R. Bug, S.A. Safran and I. Webman; Phys. Rev. Lett. **54**, 1412 (1985)