PHYSICAL REVIEW B VOLUME 37, NUMBER 4 1 FEBRUARY 1988

Nonuniversal behavior of the cluster properties in continuum systems

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(Received 31 July 1987; revised manuscript received 5 November 1987)

Monte Carlo simulations on the inverted-random-void model show that there is a fundamental difference between the critical behavior of lattices and simple continuum systems. This difference is not only manifested in the transport properties but also in the geometrical-statistical properties. In particular, while the mean cluster-size exponent is universal, the corresponding amplitude ratio is not.

Until recently it was generally believed that continuum percolation[1] and lattice percolation[2] show the same critical behavior.[3-8] It was pointed out then that, although the well-known geometrical-statistical critical exponents, β, γ, τ, and ν, are the same for the two groups of systems,[3-8] the critical exponents of the transport properties[9] are not necessarily the same. This finding was interpreted[9] as indicating that while the bond connectivity of the lattice and the continuum are the same, the continuum may also have a bond-strength distribution. Such a distribution has an effect only on the transport properties. As a representative model of the behavior of many continuum systems[10] it appears useful to consider one for which both the geometrical-statistical exponents and the transport exponents have been discussed previously. Such a continuum system is that of permeable objects[8] which recently became known as the inverted-random-void[9,11] model (see below). For this three-dimensional system, the conductivity exponent is the same as that of lattices, whereas the permeability and elasticity exponents are different than those of lattices.[9] On the other hand, studies of the critical behaviors of the geometrical-statistical properties of this system yielded universal values for the corresponding exponents.[3,8]

Considering the above geometrical-statistical and transport properties, one is led to the fundamental question of whether transport properties are the only manifestation of the difference between the critical behavior of continuum and lattice systems. For instance, is the above-mentioned conjecture of a universal behavior of the connectivity[8,9] justified? Since we already know that the critical geometrical-statistical exponents are the same, such differences, if they exist, should appear in more subtle observables of the systems. Hence, in searching for possible differences between continuum percolation and lattice percolation one has to examine observables other than the critical exponents.

A hint that such a difference exists was provided recently[12] by the determination of a critical amplitude ratio of a two-dimensional continuum system of bonds. In the corresponding model the probability for the existence of a bond has a Gaussian decrease with increasing distance between corresponding random sites. This rather special model, however, does not yield a direct indication regarding simple geometrical-continuum systems in general, and the many conventional continuum systems made of objects[13] in particular. Furthermore, at present, it is not apparent from that special model to what extent its simple random geometry determines the nonuniversal amplitude ratio and how one should model the transport in such a system. Nonetheless, that work,[12] in which the mean cluster-size amplitude ratio[14] R was determined, has motivated us to examine the same quantity[15] for the inverted-random-void model in order to determine whether geometrical-statistical universality is obeyed in simple and well-known continuum systems.

In the inverted-random-void model,[8,9] permeable objects are randomly distributed in space. Two of them are considered to be in contact if there is some overlap between them, and the onset of percolation is determined by the formation of a continuous path of intersecting objects across the sample. The Monte Carlo algorithm for the derivation of the geometrical-statistical properties of this model has been described earlier.[8] Here, however, we have done the computations both above and below the percolation threshold N_c (the critical concentration of permeable objects above which percolation exists). Briefly, the density of the sample is increased by increasing the number of objects N in a unit cube. The "measurements"[8] consist of correspondingly following various quantities[2] such as $n_s = N_s/N$ (where N_s is the number of clusters of size s) or the mean cluster size (known also as the percolation susceptibility):

$$\chi = {\sum}' s^2 n_s \ . \tag{1}$$

The fact that this sum excludes the spanning cluster is one reason for the few data available (even for lattices) for χ in the range $N > N_c$, where this exclusion considerably reduces the ensemble on which the statistics is performed. In the system under discussion one expects then the behavior:[2,12]

$$\chi = C_-(1 - N/N_c)^{-\gamma} \text{ for } N < N_c \tag{2}$$

and

$$\chi = C_+(N/N_c - 1)^{-\gamma} \text{ for } N > N_c \ . \tag{3}$$

If universality prevails, both γ and $R = C_-/C_+$ of the present continuum system should be the same as those found for lattice models.[12,14]

The most commonly studied inverted random-void system is that of spherical objects.[7-9] We have thus examined this system by considering four different samples (different pseudorandom generator initiation seeds) of three-dimensional spheres of radius $r=0.025$ (where the lengths are given as fractions of the edge length of the unit cube in which the permeable objects are randomly implanted[8]). The percolation thresholds for this radius were between $N_c=5250$ and $N_c=5580$ for the four samples. The results (apart from the deviations at very low and very high $|N/N_c-1|$ values, see below) were much the same for the four samples. Hence, we show typical results obtained on one of the samples in Fig. 1. It is clearly seen in this figure that a power-law behavior is a very good description of the $N<N_c$ data points. Indeed, a least-squares fit[8] to these points yields the known lattice exponent of $\gamma=1.9\pm0.1$. As expected, the quality of the data for the $N>N_c$ data points is much poorer (see above). Nonetheless, it appears very reasonable that, except for the very low and very high values of $|N/N_c-1|$, the power law is the same as that of the $N<N_c$ data. This is illustrated by the dashed line which is intentionally drawn parallel to the solid line. The deviations at the extremes of the log $(|N/N_c-1|)$ range are not unexpected,[2,12] since finite-size effects are well known to smear the divergent behavior close to N_c and correction to scaling terms become important far from N_c. At present, it is not clear whether it is the latter effect or the poor statistics of the cluster sizes for $N\approx 2N_c$, which is responsible for the apparent saturation of the data points at this end. We

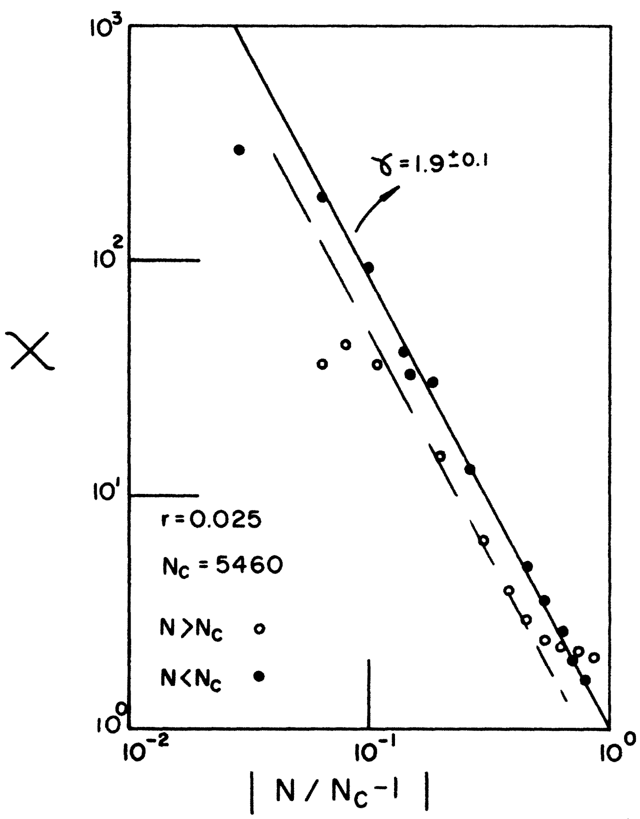

FIG. 1. A typical dependence of the mean cluster size on the proximity to the percolation threshold for a system of permeable spheres. The solid line represents the best fit to the data points for $N<N_c$, from which the value of γ is derived.

should point out that this effect is found in all our simulations. In the present work, however, we are interested in the amplitude ratio R for the range where the universal exponent γ appears to determine the $\chi(|N/N_c-1|)$ dependence. The value of R did not exceed 2 in any of the samples. Hence, one may conclude that $1\leq R\leq 2$. The important point of course is that R is not only an order of magnitude smaller than the values obtained for lattices,[16,17] but that it is also smaller than the lowest estimate of direct ϵ expansion[14] ($R=2.7$).

Since the purpose of this paper is to show the remarkably smaller value of R for a simple geometrical-continuum system, in comparison with values obtained for lattices, no further effort was made here to improve the numerical or statistical quality of the results and no attempt was made to study the finite-size effects. To do all this one has to use larger samples that are beyond our ability at present. In particular, one notes that statistics of many smaller samples will not be too helpful in the present case. This is a consequence of the fact that the range of scaling behavior for $N>N_c$ will be further reduced, and thus the R values to be derived, will be associated with less than the one order of magnitude N/N_c-1 range which was studied here. Correspondingly, a quantitative study of finite-size effects will also require larger samples. In fact, the small value of R in the continuum is the reason for our ability to study χ for $N>N_c$ in the relatively small samples used here. In lattices, because of the large R values, samples with similar N's will yield a completely smeared behavior of χ over the $N>N_c$ range studied here. Indeed, much larger samples are required for the same study in lattices. As pointed out above, this is probably the reason for the very few previous χ studies[16,17] of lattices in the $N>N_c$ range.

To emphasize the above point, and to show that in the continuum R is system dependent, we have carried out similar simulations on four samples in which the objects had the shape of capped cylinders[8] (of length L and radius r). Typical results on such a sample are shown in Fig. 2. It appears now that within the accuracy of the present results $R=1$. The largest possible R value obtained on the other three samples did not exceed 1.5. Hence, it seems well established that the R is system dependent in the continuum and is much smaller, at least for the inverted random-void model, than values expected from universality.[14,16,17]

Since the R values appear to decrease with the aspect ratio of the object, and since in two dimensions the lattices' R value[16,17] is of the order of 200, it appears reasonable to expect that a dramatic decrease of R will be found for a system of elongated two-dimensional objects. Correspondingly, we have carried out the same kind of Monte Carlo computation on a two-dimensional system of permeable "widthless sticks"[18] of length L. Typical results of such a simulation are shown in Fig. 3. Here, it is clearly seen that the expected γ value (2.45 ± 0.08) is obtained and that R is of the order of 3. This R value is indeed dramatically smaller than the above-quoted result for lattices. It is also smaller than the values found for the random system of Ref. 12 and is of the order of the lowest ϵ expansion estimate ($R=3.6$).

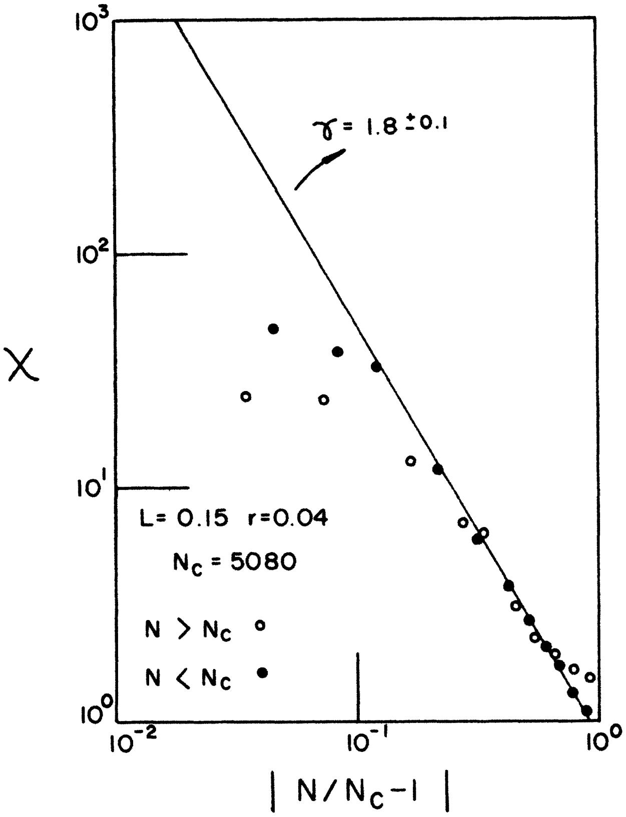

FIG. 2. Same as Fig. 1 except that the system consists of permeable capped cylinders.

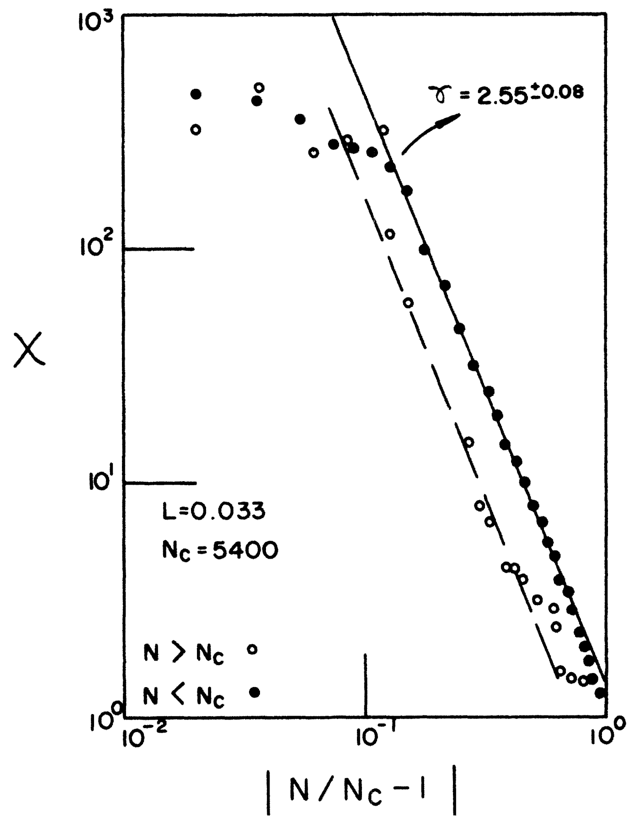

FIG. 3. Same as Fig. 1 except that a two-dimensional system of permeable widthless sticks is considered.

All the above results show that simple continuum systems differ from their lattice counterparts in the critical behavior of their geometrical-statistical properties. While the growth rate of the mean cluster size (which is characterized by the exponent γ) is the same as that of lattices, the relative importance of the spanning (or percolating) cluster is much smaller in continuum systems. This is manifested by the fact that C_+ stays of the order of C_- through the onset of percolation. It appears that the present results have to do then with a more "open" structure of the spanning clusters in continuum systems. This suggestion is supported by the effect of the high aspect ratio on both R and B_c, where B_c is the critical number of bonds per site at the onset of percolation.[19] Both quantities decrease with increasing aspect ratio, which means that a "lower connectivity" and thus a relatively smaller number of spanning cluster elements is required for the formation of a spanning cluster. This conclusion seems to suggest a correlation between the percolation threshold and the amplitude ratio R. It will be interesting to check this correlation under the variation of other parameters which characterize the continuum system. For example, the variation in the hard-core (radius b) to soft-shell (thickness a-b) ratio[20,21] or the introduction of interactions[20] is expected to yield similar correlations. Our preliminary computations on a three-dimensional system of semipermeable spheres ($N_c \cong 1400$) indicate that this will be the case, since for $b/a = 0.75$ our largest R value was 1.3. However, as mentioned above, larger samples will be needed in order to establish a quantitative relation between R and b/a.

It is interesting to compare the present results with those obtained for a kinetic gelation model[22] which was built on a cubic lattice. The R values obtained there are of the same order of the values obtained here, and these values decrease with decreasing percolation threshold. (The parameter used for the variation was the concentration of initiators[22].) In addition, the fact that in our purely geometrical system and in the kinetic gelation model the exponents found were the universal ones may indicate that both the continuum geometrical system and the kinetic gelation model belong to the same universality class. More detailed studies and attempts to map one system onto the other are necessary, however, to confirm or disprove this indication.

In conclusion, we have shown that the amplitude ratio of a geometrical-statistical property of simple percolating continuum systems is substantially different from that of lattices. It is found that the importance of the spanning cluster is significantly smaller in continuum systems, and that the relative importance depends on the details of the system. Combining these observations and the nonuniversality of the transport properties, one concludes that only the geometrical-statistical exponents can be considered the same (i.e., universal) for all lattice and continuum systems.

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