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Universality of continuum percolation

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We study by Monte Carlo simulation the universality of continuum percolation for randomly centered disks and spheres. We specifically consider the amplitude ratio of susceptibilities C_-/C_+ which is supposed to be universal but found to be different from the lattice value. Our data, however, indicate no clear evidence of such a nonuniversal behavior as long as the finite-size effects are taken into account. We also present simulation data for continuum percolation of the penetrable-concentric-shell model.

Until recently it has been common to use lattice models in discussions of percolation in real materials.[1,2] More recently, investigators have focused their attention on continuum models of percolation since such models are better able to capture the essential physics in real systems. It was relatively recently that the question regarding the universality of continuum and lattice percolation was addressed. In the prototypical continuum percolation model, randomly centered particles are distributed in space and a bond is assumed to exist between two such particles if they overlap. Various numerical studies indicated that all statistical critical exponents for continuum percolations of overlapping disks and spheres are the same as for lattice percolations.[3-5]

In contrast to this, however, it has been reported that the amplitude ratio of susceptibilities, defined by $R = C_-/C_+$, which is supposed to be universal, is different from the lattice value.[6] Here C_- and C_+ are the amplitudes of susceptibilities below and above the percolation threshold p_c. A hint that such a difference exists was provided recently by the determination of the amplitude ratio for two-dimensional continuum percolation of random bonds.[7] While the lattice value of R is about 200,[8] the observed value for such a model was at least one order smaller than this. Motivated by this, Belberg[6] has carried out Monte Carlo simulations for overlapping spheres, capped cylinders, and (two-dimensional) widthless sticks. He obtained R to be less than two for three dimensions and of the order of three for two dimensions. These are evidently one or two orders smaller than lattice values, where the known lattice values are $R \simeq 196$ and 11 for two and three dimensions, respectively.[8] Similar difference was also observed previously. For example, Gawlinski and Stanley[3] used a certain definition of susceptibility and obtained R to be about 50 for freely overlapping disks. From these observations, it is concluded that the universality prevails *weakly*, in the sense that only the statistical critical exponents are the same for lattice and continuum systems, while the amplitude ratio remains different.

The unexpectedly small values of R might be due to the different definitions of susceptibility. The susceptibility is defined in the theory of percolation by two alternative ways:

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

and

$$S = \sum_s{}' n_s s^2 \Big/ \sum_s{}' n_s s \,, \tag{2}$$

where n_s denotes the mean number of clusters of size s per particle and the prime implies that the biggest cluster is excluded in the sum for $p > p_c$. The former is usually called "susceptibility" and the latter often "mean cluster size." In the limit of the infinite system, both χ and S are expected to show the same critical behavior; however, for any finite-sized system, the asymptotic behavior of one is different from another. To see this clearly, let $n_s = N_s/N$, where N_s is the number of clusters of size s and N is the total number of particles. Then, Eqs. (1) and (2) can be written, respectively, as

$$\chi = \frac{1}{N} \sum_s{}' N_s s^2 \tag{3}$$

and

$$S = \frac{1}{N'} \sum_s{}' N_s s^2 \,, \tag{4}$$

where $N' = \sum_s' N_s s$. For $p < p_c$, N' is simply the total number of particles in the system and both Eqs. (3) and (4) are the same. For $p > p_c$, on the other hand, N' is the number of particles which are not members of the largest cluster and thus, smaller than N. Therefore, Eq. (4) is greater than Eq. (3), indicating that the amplitude of S is greater than that of χ. It is thus clear that the two definitions yield different values of R for any finite-sized system. As the concentration increases, the finite clusters above p_c tend to be connected to the largest cluster. For sufficiently high concentrations the remaining finite clusters are those of, at most, few particles, and therefore, χ and S approach, respectively, to $1/N$ and 1 as $p \rightarrow 1$. This kind of saturation on unity for S was observed in Monte Carlo data by Belberg.[6] Although he claimed that Eq. (1) was employed in his simulation, we believe that such saturation is due to the mean-cluster-size definition given in Eq. (2). (Note that what he called mean cluster size is our susceptibility function.)

The small values of R for the mean-cluster-size function were already found for lattice percolation.[8,9] While the susceptibility function in two dimensions gives R to be about 200, estimated from the mean cluster size was an order of unity by series analysis[10] and about 20 by Monte

Carlo simulations.[8,9] Because of these inconsistent values, one must determine which definition is to be used for scaling analysis. Nakanishi and Stanley[11] have pointed out that setting $\gamma(p>p_c)=\gamma(p<p_c)$ leads to results with an anomalous behavior in S for $p>p_c$, while no such anomaly occurs in χ. The source of such an anomaly is evidently an extra singularity introduced by the denominator in S; $\sum_s' n_s s \sim p(1-P_\infty)$, where P_∞, the percolation order parameter, is known to scale as $P_\infty \sim (p-p_c)^\beta$. Above p_c, the factor $(1-P_\infty)$ gives a correction term $1+O[(p-p_c)^\beta]$, which makes numerical extrapolation at finite values of $p-p_c$ very difficult. Indeed Hoshen *et al.*[8] have found by Monte Carlo simulations that the exponent γ determined from the mean-cluster-size function above p_c had an unacceptably small value of 1.9 in two dimensions. This is quite similar to the situation in the series results, where it was not possible to determine γ reliably above p_c.[10] By these reasonings, Nakanishi and Stanley[11] suggested that the susceptibility function be used.

In this Rapid Communication we present Monte Carlo simulation results of the amplitude ratio of susceptibility for continuum percolation of freely overlapping disks and spheres. We obtained R to be about 192 and 19 for two and three dimensions, respectively. These values are reasonably close to the known lattice values, and thus, our data do not indicate a clear evidence of a nonuniversal behavior in R, unlike the work of Belberg.[6] We also present the simulation data for the penetrable-concentric-shell (PCS) model.[12] In the PCS model, each sphere (disk) of radius $\sigma/2$ (where we have let $\sigma=1$) is composed of an impenetrable core of radius $\lambda\sigma/2$, encompassed by a perfectly penetrable shell of thickness $(1-\lambda)\sigma/2$. The extreme limits $\lambda=0$ and 1 corresponds, respectively, to the cases of fully penetrable and totally impenetrable particles.

The susceptibility function χ defined in Eq. (1) was calculated for overlapping disks and spheres as a function of reduced number density η [defined by $\eta=(N/L^D)V_1$, where V_1 is the volume of each D-dimensional sphere] for several values of the size of system L; $L=30$, 40, and 50, and $L=15$, 18, and 20 for two and three dimensions, respectively. The periodic boundary conditions were employed to minimize the finite-size effect. The percolation threshold η_c was set as a parameter and selected in such a way that χ below and above η_c show power law with the same exponent. Plotted in Fig. 1 are the data for overlapping spheres averaged over 100 realizations, using $\eta_c=0.3480$ (cf. $\eta_c\simeq 0.35$ by Monte Carlo simulations[13]). For $\eta<\eta_c$, data are similar to the previous Monte Carlo data;[6] however, for $\eta>\eta_c$ our data show much smaller amplitude, indicating a larger amplitude ratio. The major difference is that our data are free of the apparent saturation which was found in all data in the previous work.[6] This supports our assertion that the mean-cluster-size function instead of susceptibility has been employed in Ref. 6. The critical exponent γ and the amplitude ratio R were estimated from the plot; $\gamma=1.91\pm0.01$ and $R=19\pm1$, where the quoted errors are those associated with linear regressions and there may be additional statistical errors not accounted for. The value of γ is reasonably close to the lattice value ($\gamma\simeq1.8$, cf. Ref. 14) and is

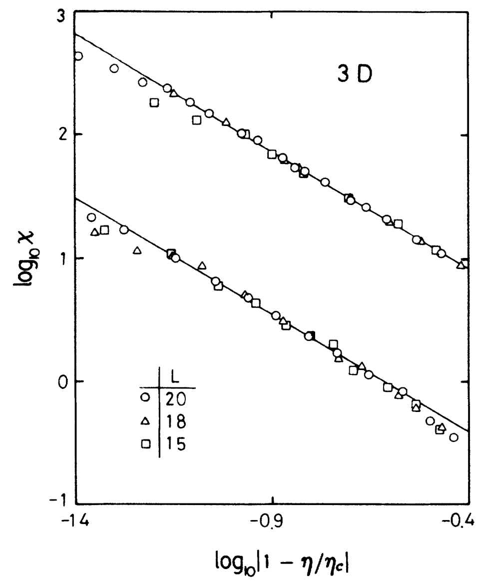

FIG. 1. Double logarithmic plot of susceptibilities for continuum percolation of overlapping spheres. The percolation threshold used is $\eta_c=0.3480$.

also close to the previously measured continuum value.[6] On the other hand, our estimate of R appears to be somewhat large compared to the lattice value;[8] however, it is not one or two orders different from it, unlike the work of Belberg.[6] [Note that our data are at least 1 order of magnitude higher statistics than in Ref. 6.] It is thus certainly unfair to conclude, without taking into account the finite-size effect, the "nonuniversality" of the amplitude ratio of susceptibilities. In fact, considering the two-dimensional result (see below), we believe that R is also universal for continuum percolations of overlapping disks and spheres.

Plotted in Fig. 2 are the data for overlapping disks aver-

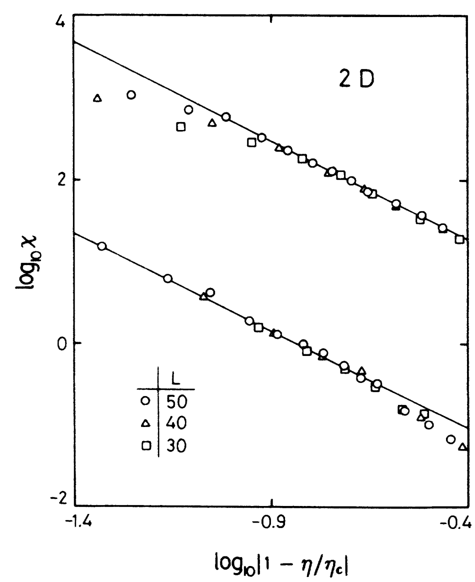

FIG. 2. Double logarithmic plot of susceptibilities for continuum percolation of overlapping disks. The percolation threshold used is $\eta_c=1.1314$.

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aged over 200 realizations. Data again show very good power law both below and above η_c, using $\eta_c = 1.1314$, for a wide range except for the two extreme limits of η, where the finite-size effect is known to smear the divergent behavior. The least-squares fit to the data in the linear region yields $\gamma = 2.39 \pm 0.02$ and $R = 192 \pm 20$. The estimate of γ is again close to the lattice value ($\gamma = \frac{43}{18}$, cf. Ref. 1) and also close to the previous Monte Carlo estimate[3] for the continuum system. The amplitude ratio R is also reasonably close to the known lattice value $R \simeq 197$.[8] This is a good indication that the amplitude ratio of susceptibilities for continuum percolations of overlapping particles are the same as for lattice percolations, and thus, they belong to the same universality class even when the amplitude ratio is considered.

For random bond percolation, however, the susceptibility definition yielded a smaller amplitude ratio in Ref. 7. Since the connectivity rule defined for such a model is different from that for the standard continuum percolations of overlapping particles, our work does not rule out the possibility of nonuniversal behavior in R between such model and lattice percolations. The kinetic gelation[15] and the *AB* bond percolations[16] are similar cases, but we claim that the continuum percolations of overlapping particles are not such cases.

We have also carried out Monte Carlo simulations for the PCS model for $0 < \lambda < 1$ for both two and three dimensions. A conventional Metropolis algorithm[17] was employed to generate equilibrium realizations and the susceptibility was calculated for several selected values of λ as a function of η.

Data for $L = 20$ and $\lambda = 0.6$ and 0.8 for three dimensions, averaged over 100 realizations, are compared in Fig. 3 with those of overlapping spheres. The parallel lines were obtained using $\eta_c = 0.3196$ and 0.3396 for $\lambda = 0.6$ and 0.8, respectively. As λ increases, the susceptibilities both below and above η_c seem to decrease. The source of this effect is the short-ranged repulsive interactions, which in general appears to force particles apart and form clusters of relatively smaller sizes. Estimates of γ from the plot are $\gamma = 1.84 \pm 0.02$ for $\lambda = 0.6$ and $\gamma = 1.79 \pm 0.02$ for $\lambda = 0.8$. These values are slightly smaller than, but still reasonably close to, our estimate for overlapping spheres. As λ increases, γ in general seems to decrease slightly; however, the difference appears to be within statistical errors. (Note that errors quoted are those associated with linear regressions.) The estimates of R, $R = 18.1 \pm 1.1$ for $\lambda = 0.6$ and $R = 22.3 \pm 1.6$ for $\lambda = 0.8$, are also close to that for overlapping spheres, indicating that the hard-core repulsion does not affect significantly the critical behavior in three dimensions.

In Fig. 4, data for two dimensions for $L = 50$ and $\lambda = 0.3$ and 0.7 are compared similarly with those for overlapping disks. The estimates of γ are $\gamma = 2.41 \pm 0.03$ for $\lambda = 0.3$ and $\gamma = 2.38 \pm 0.02$ for $\lambda = 0.7$, which are again close to that for overlapping disks. On the other hand the amplitude ratios estimated from the plot, $R = 381 \pm 20$ for $\lambda = 0.3$ and $R = 615 \pm 60$ for $\lambda = 0.7$, are considerably greater than our estimate for overlapping disks, and, moreover, R seems to depend upon λ. This is rather surprising because we obtained γ for all considered values of λ very close to the overlapping particles for both two and three dimensions and, in addition, the amplitude ratio in three dimensions was also estimated to be similar even for relatively large hard-core volume fractions. One possible way to explain such large values of R is to assume that the finite-size effect is dependent upon λ, i.e., the finite-size effect becomes important as λ increases. The η_c^{eff} which was used in our data analyses is, in general, deviated from the true percolation point η_c^{true} and the deviation $\Delta\eta_c = |\eta_c^{\text{eff}} - \eta_c^{\text{true}}|$ is expected to diminish as the size of the system increases. The comparison of $\Delta\eta_c$ for different values of λ seems to indicate that the finite-size effect indeed becomes important as λ increases. Using the recent accurate determinations of η_c,[18] $\Delta\eta_c$ can be estimated as $\Delta\eta_c \simeq 0.01$ for both $\lambda = 0.3$ and 0.7, while that for

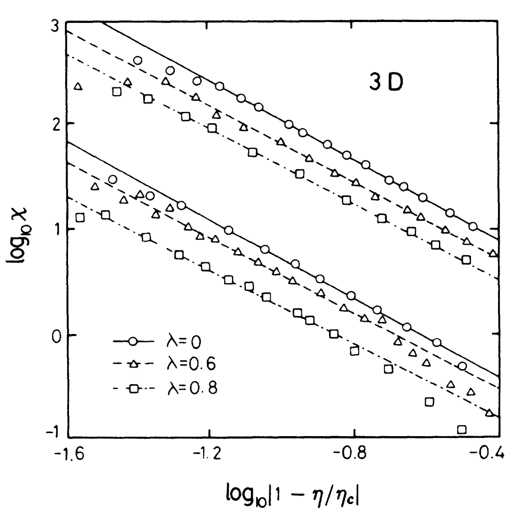

FIG. 3. Double logarithmic plot of susceptibilities for the three-dimensional PCS model for $\lambda = 0.6$ and 0.8, compared to those of overlapping spheres ($\lambda = 0$). The percolation thresholds used are $\eta_c = 0.3196$ and 0.3396 for $\lambda = 0.6$ and 0.8, respectively.

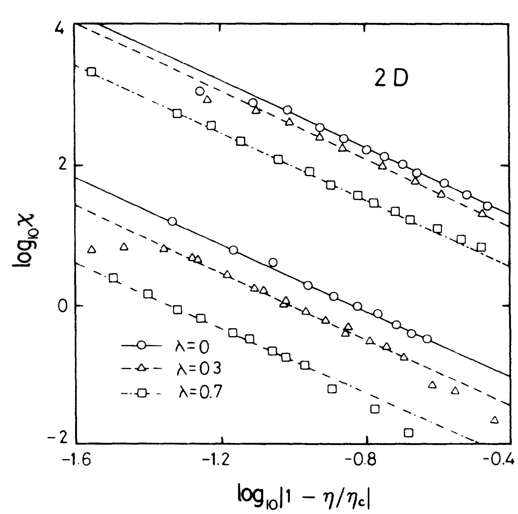

FIG. 4. Double logarithmic plot of susceptibilities for the two-dimensional PCS model for $\lambda = 0.3$ and 0.7, compared to those of overlapping disks ($\lambda = 0$). The percolation thresholds used are $\eta_c = 0.9932$ and 0.7792 for $\lambda = 0.3$ and 0.7, respectively.

$\lambda = 0$ is only about 0.003. Clearly $\Delta\eta_c$ increases as λ increases even though we used the same size system $L = 50$ for all three cases of λ. Another possibility one can think of is that such increases of R as λ increases might be a precursor to a crossover from the extreme of $\lambda = 0$ (fully penetrable case) to a different universality class at $\lambda = 1$ (impenetrable, hard-particle system). If we consider the mean cluster size for the hard-particle system, it would be precisely 1 for $\eta < \eta_c$ because the probability of having two particles in contact is exactly zero, while that at close-packing volume fractions diverges suddenly, suggesting a possible large increase in either γ or R. The recent work[19] for continuum percolation of short-ranged potential also appears to strengthen the latter postulate.

In any of these cases, however, similar behavior should be observed for three dimensions as well. As we have already seen, such a large increase in R was not a characteristic for the three-dimensional PCS model.

In summary, we have studied by Monte Carlo simulation the susceptibilities of continuum percolation for overlapping spheres and disks and for the PCS model for several selected values of λ between 0 and 1. For overlapping particle systems, we found that the amplitude ratios of susceptibilities were similar to the lattice values, indicating a *strong* universality between lattice and continuum percolations. For the PCS model for intermediate λ, we found the susceptibility exponents similar to the fully penetrable cases for both dimensions. The amplitude ratio R in three dimensions was also found to be close to the overlapping sphere system. On the other hand, in two dimensions, it seems to be considerably greater than (though, of the same order as) that of the overlapping disks. We discussed some possible causes of such large increases.

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