Scaling behavior of diffusion on percolation clusters

S. Havlin, D. Ben-Avraham, and H. Sompolinsky

Department of Physics, Bar-Ilan University, Ramat-Gan, Israel

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A scaling analysis is performed on Monte Carlo simulations of random walks on percolation clusters both above and below the threshold p_c. The average diffusion constant is described by a single scaling function in which the crossover from an algebraic decay (in time) near p_c to the asymptotic behavior above or below it occurs at time $t_{\text{cross}} \propto |p - p_c|^{-(2\nu - \beta + \mu)}$. The value of the percolation conductivity exponent μ is found to be 1.05 ±0.05 for two-dimensional systems and 1.5 ±0.1 for three dimensions.

Diffusion near the percolation threshold of randomly diluted conducting networks has been of considerable interest in recent years.[1-7] In the conducting phase $(p > p_c)$, the *average* diffusion constant

$$D_a(t,p) \equiv \langle R^2(t) \rangle_a / t$$

of a random walk $R(t)$ on the network is finite in the long-time $(t \to \infty)$ limit. Its value in that limit is proportional, via the Einstein relation, to the dc conductivity $\sigma(p)$ of the network. Indeed, following a suggestion by de Gennes, computer simulations of diffusion on percolation lattices have been used[2,3] to determine the conductivity exponent μ via

$$D_a(t \to \infty, p) \propto \sigma(p) \propto (p - p_c)^\mu, \quad p > p_c \ . \quad (1)$$

However this behavior holds only in the neighborhood of p_c and in very long times such that the average span $R_a \equiv (\langle R^2(t) \rangle_a)^{1/2}$ of the walks is much larger than the percolation correlation length ξ. On the other hand, when $R_a \ll \xi$ one expects a behavior which is similar to that of a diffusion at the threshold p_c, where it was recently shown[7] that D_a vanishes algebraically with time,

$$D_a(t, p_c) \propto t^{(2 - D')/D'} \ . \quad (2)$$

The exponent D' defines the scaling of distances along the walk with time, i.e., $R_a^{D'} \propto t$ at p_c. The result (2) was recently confirmed by Ben-Avraham and Havlin[7] through computer simulations of random walks at $p = p_c$, which also yielded the estimate $D' = 2.76 \pm 0.05$ for $d = 2$ and $D' = 3.9 \pm 0.1$ for $d = 3$. In practice the condition $R_a \gg \xi$ is hardly achieved in simulations near p_c. This limits the reliability of determining μ through Eq. (1) and calls for a method which will incorporate the crossover from a finite diffusion constant above p_c, Eq. (1), to the behavior at criticality, Eq. (2).

In this work we present the results of computer simulations of random walks on percolation clusters near the percolation threshold. The results are stud-ied on the basis of a scaling function which, we assume, governs the diffusion properties throughout the critical regime ($|1 - p/p_c| \ll 1$) for both short and long length scales. This scaling form has also been proposed recently by Gefen *et al.*[6] Both the scaling ansatz and the resulting scaling relations are obeyed quite well by the numerical data, thus supporting the physical assumptions about the scaling properties near the percolation threshold. In addition, since the scaling function is valid in all time scales, by using all the available numerical data we are able to extract a relatively reliable numerical estimate of the value of the conductivity exponent μ.

Results are presented for both the diffusion $\langle R^2(t) \rangle_a$ which is averaged over all percolation clusters as well as for the diffusion $\langle R^2(t) \rangle_l$ which is constrained to clusters that are much *larger* than the span of the diffusion. It is hoped that this will clarify the relationship between the diffusion in each of these averages and other percolation exponents.

We consider first the average diffusion constant D_a. For $p > p_c$ and $R_a \gg \xi$ (i.e., $t \to \infty$), Eq. (1) is expected to hold. for $p < p_c$ and $t \to \infty$, the dominant contribution to $\langle R^2(t) \rangle_a$ comes from clusters whose (linear) size is equal to or bigger than $\xi \propto |p - p_c|^{-\nu}$. In each of these clusters $R^2(t) \propto \xi^2$, but the probability of being on one of these big clusters is, by the usual percolation scaling assumptions,[8] proportional to $|p_c - p|^\beta$. Thus the average diffusion constant behaves below p_c as

$$D_a(t \to \infty, p) \propto t^{-1}(p_c - p)^{-2\nu + \beta}, \quad p < p_c \quad (3)$$

as noted by Stauffer.[8] We now combine the results (1)–(3) in the following scaling form,

$$D_a(t,p) = t^{2/D' - 1} f_a((p/p_c - 1) t^{(D' - 2)/\mu D'}) \ , \quad (4)$$

where

$$f_a(x \to \infty) \propto x^\mu \ , \quad f_a(x \to -\infty) \propto (-x)^{-2\nu + \beta} \ ,$$

and

$$f_a(x \to 0) = \text{const} .$$

Consistency with Eq. (3) yields the additional relation

$$D' = 2 + \frac{\mu}{\nu - \beta/2} . \tag{5}$$

Thus the crossover time from the behavior (1) or (3) to that of (2) occurs at

$$t_a \simeq |p - p_c|^{-\mu D'/(D'-2)} = |p - p_c|^{-(2\nu - \beta + \mu)} .$$

We now present numerical evidence for the scaling relation (4) for diffusion which is averaged over all percolation clusters. The diffusion was performed by a new efficient Monte Carlo method. Each walk starts from a site (the origin) which is assumed to belong to a cluster. Then the nearest neighbors (NN) of the origin are chosen to be occupied (empty) with a probability p $(1-p)$. The walk diffuses randomly to one of the occupied NN sites. Then, the occupation of each of the NN of the latter site is determined with a probability p, unless of course its occupation has been already determined in an earlier step. The random walk is continued in this fashion up to the desired number of steps. Thus, each diffusion is per-

formed on a different cluster. By this method we construct and store only those parts of the cluster which are in the neighborhood of the walk.

We have studied $D_a(t,p)$ for about 5×10^3 diffusions in the range $|1 - p/p_c| \leq 0.2$ on percolation clusters embedded on square $(d=2)$ and simple cubic $(d=3)$ lattices. We reached a maximum diffusion time of 1600 steps for $d=2$ and of 640 steps for $d=3$. To increase the statistics, at each walk we have averaged $R^2(t)$ over the distances between all pairs of sites on the walk which are separated by t steps.[9] In Fig. 1 we present for the $2d$ case the best fit of the data to a scaling function of the form (4) achieved by varying μ and D'. Figure 2 presents the same analysis for $d=3$. The numerical estimates obtained for the exponents are $D'=2.85 \pm 0.05$, $\mu = 1.05 \pm 0.05$, for $d=2$ and $D'=3.9 \pm 0.1$, $\mu = 1.5 \pm 0.1$, for $d=3$. These values, together with the known estimates[8] for ν and β, are in good agreement with Eq. (5) (see Table I).

We now turn to the diffusion constant D_l of walks on clusters which are much *larger* than the span of the walks. Since the probability of being on clusters with sizes which are equal to or bigger than ξ behaves as $|p - p_c|^\beta$ both above and below p_c, it is expected that (a) for $p > p_c$ and $R_l = (\langle R^2 \rangle_l)^{1/2}$
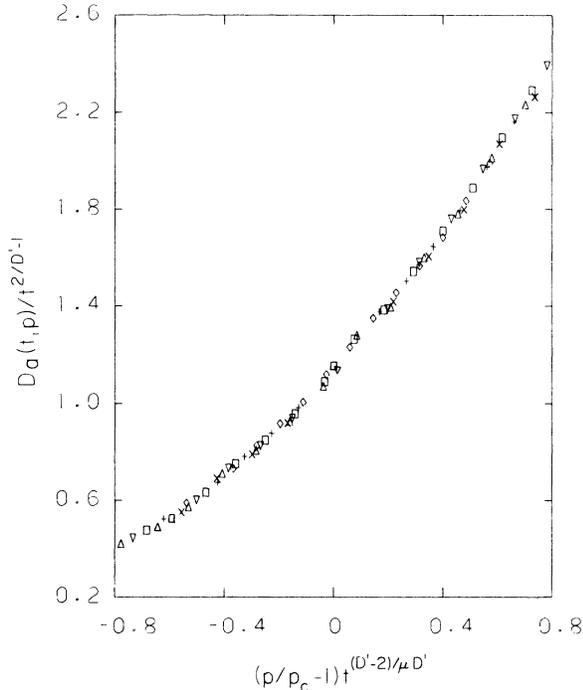

FIG. 1. Monte Carlo results of diffusion on percolation clusters in a two-dimensional square lattice. Results are presented in the scaling form Eq. (4). The symbols mark different time lengths as follows: □ corresponds to 300 steps; + to 500; □ to 700; ∇ to 900; Δ to 1100; and × to 1300 steps. Concentrate p varies in the range $|p/p_c - 1|$ ≤ 0.15 and $p_c = 0.593$.
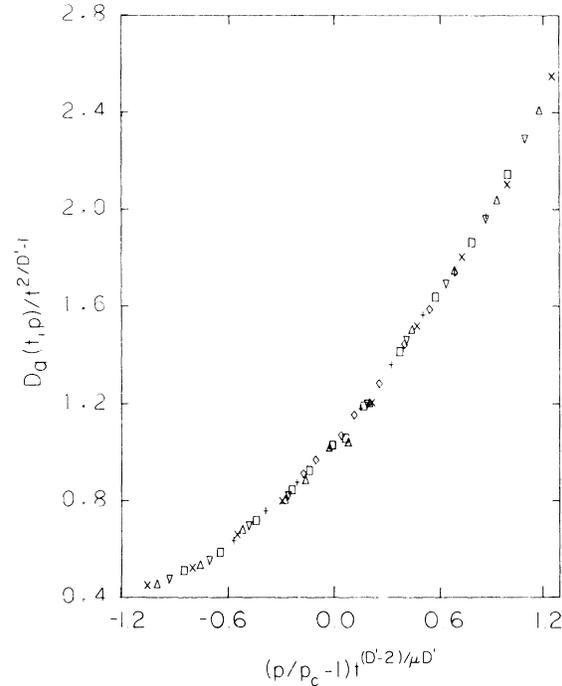
FIG. 2. Monte Carlo results of diffusion on percolation clusters in a three-dimensional simple cubic lattice. Results are presented in the scaling form Eq. (4). The symbols mark different time lengths as follows: □ corresponds to 100 steps; + to 200; □ to 300; ∇ to 400; Δ to 500; and × to 600 steps. Concentration p varies in the range $|p/p_c - 1|$ ≤ 0.2 and $p_c = 0.311$.

TABLE I. Critical exponent of diffusion on percolation.

d	D'	Present work D	μ	$\mu - \beta$	μ	β	ν
2	2.85 ±0.05	2.7 ±0.05	1.05 ±0.05	1.00 ±0.05	0.9−1.5[a]	0.14 ±0.02[b]	1.33 ±0.05[b]
3	3.9 ±0.1	3.35 ±0.1	1.5 ±0.1	1.2 ±0.1	1.6−1.95[a]	0.4 ±0.05[b]	0.85 ±0.05[b]

[a]From Table I in Ref. 5.   [b]From Ref. 8.

$\gg \xi$, $D_l \propto (p-p_c)^{\mu-\beta}$; (b) for $p < p_c$ and $t \to \infty$, $D_l \propto t^{-1}|p - p_c|^{-2\nu}$; and (c) for $R_l \ll \xi$, $D_l \propto t^{2/D-1}$. The scaling function of D_l which is consistent with these properties is

$$D_l(t,p) = t^{2/D-1}f_l((p/p_c-1)\,t^{(D-2)/(\mu-\beta)D}) \quad , \quad (6)$$

where

$$f(x \to +\infty) \sim x^{\mu-\beta} \quad ,$$

$$f(x \to -\infty) \sim (-x)^{-2\nu} \quad ,$$

$$f(x \to 0) = \text{const}$$

and consistency requires

$$D = 2 + \frac{\mu - \beta}{\nu} \quad . \quad (7)$$

The result (7) was first given by Alexander and Or-bach.[4] It yields together with (5) the ratio D/D' $= 1 - \beta/2\nu$ which was also derived by Ben-Avraham and Havlin.[7] Note that the crossover time

$$t_l \sim (p - p_c)^{-(\mu-\beta)D/(D-2)}$$

of D_l is equal to that of D_a since $(\mu-\beta)D/(D-2)$ $= \mu D'/(D'-2) = 2\nu - \beta + \mu$.

The scaling form (6) was checked by computer simulation of diffusion on clusters (prepared by the cluster growth method)[10] which were much larger than the span of each walk. We have studied $D_l(t,p)$ for about 10^3 percolation clusters, performing 10 diffusions of length of 640 steps on each cluster, for the square ($d=2$) and the simple cubic lattice ($d=3$). The results are quite similar to those of Figs. 1 and 2. It should be noted, however, that below p_c it is difficult to create large clusters and therefore the statistics are poorer in this region. The best scaling fit is obtained using the numerical values $D = 2.7 ±0.05$, $\mu - \beta = 1.00 ±0.05$ for $d=2$, and

$D = 3.35 ±0.1$, $\mu - \beta = 1.2 ±0.1$ for $d=3$. The results for $\mu - \beta$ are consistent with the value of μ obtained by averaging over all clusters and using the known values of β.[8] These results are also in good agreement with Eq. (7). Table I summarizes our results for the critical exponents of the diffusion on percolation. The present values of D' and D which are obtained by a scaling analysis are close to those obtained previously[7] from the measurements at $p = p_c$ by the relations $[R_a(t)]^{D'} \sim t$, $[R_l(t)]^D \sim t$. Our results for μ are close to those obtained by other Monte Carlo studies of conductivity[11] or diffusion[2] on percolation, but are lower than the estimates obtained from series expansions.[12]

In conclusion, we have shown that random walks of different lengths on percolation clusters with concentration p both above and below p_c are well described by a single scaling function which is continuous at $p = p_c$. The crossover from an algebraic decay of the diffusion constant with time near p_c to the asymptotic behavior above or below it occurs at

$$t_{\text{cross}} \propto |p - p_c|^{-(2\nu-\beta+\mu)} \quad .$$

It should be noted that the fit of the data to the scaling form was found to be quite sensitive to changes in the values of the exponents μ and D. On the other hand, even in the longest walks ($t \sim 1600$ steps) we could not fit the data to the asymptotic forms (1) or (3). The reason for this is that the spans $\sqrt{R^2}$ of our walks are never much bigger than the percolation correlation length ξ, and the crossover regime is rather wide. This was confirmed by a direct study of the properties of the percolation clusters generated in our simulations.

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