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Corrections to Scaling for Diffusion Exponents on Three-Dimensional Percolation Systems at Criticality

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Recent results of Monte Carlo simulations of the ant-in-the-labyrinth method in three-dimensional percolation lattices are reanalyzed in the light of more accurate corrections to scaling ansatz, motivated by inconsistent results that have appeared in the literature. The results are observed to be sensitive to the form of the scaling correction terms. Using a single correction term, we estimate the value $k = 0.197 \pm 0.004$ for the anomalous diffusion exponent at criticality. When two correction terms are included, $k = 0.200 \pm 0.002$ is obtained. These new estimates are consistent with known theoretical bounds, with recent series expansion results, and with numerical calculations of the conductance of random resistor networks above criticality.

KEY WORDS: Percolation; anomalous diffusion exponents; corrections to scaling.

Transport phenomena on percolation systems have been studied extensively in recent years. Of great theoretical interest is the asymptotic behavior of random walks on percolation systems at the critical concentration p_c. Such information can be related to the behavior of the conductivity of the system above p_c.[(1)]

Consider a d-dimensional lattice where the lattice sites are occupied with probability $p \geqslant p_c$, and let a walker perform a random walk between nearest neighbor occupied sites of the lattice. One can study two cases: (a) the walker starts its walk on any occupied site of the lattice, i.e., it can move either on the infinite cluster or on finite clusters, or (b) the walk is

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restricted to the infinite cluster alone. At the critical concentration p_c, the mean-square displacement of the walker is anomalous and asymptotically

$$\langle r^2(t) \rangle \sim t^{2k} \tag{1a}$$

($k < 1/2$) for case (a), and

$$\langle r^2(t) \rangle \sim t^{2/d_w} \tag{1b}$$

($d_w > 2$) for case (b). Both k and the anomalous diffusion exponent d_w are related by[1]

$$d_w k = 1 - \beta/2\nu$$

where β is the exponent for the volume fraction of the infinite network and ν is the correlation length exponent.[2] From the critical behavior of the conductivity $\Sigma \sim (p - p_c)^\mu$ near p_c, one can determine the conductivity exponent μ, which is related to d_w by[1]

$$d_w = 2 + (\mu - \beta)/\nu \tag{2}$$

The need for accurate evaluations of (1) and (2) for three-dimensional lattices has motivated much recent numerical and theoretical work. Recently, extensive Monte Carlo simulations of random walks ("ant-in-the-labyrinth" method) have been performed on randomly occupied simple cubic lattices, of up to 960^3 sites for case (a), at the critical concentration $p_c \cong 0.3116$. By using efficient vectorizable algorithms, accurate values of $\langle r^2(t) \rangle$ have been obtained.[3] To determine the asymptotic value k, however, corrections to the scaling behavior (1a) must be considered.

CASE (a)

In the third column of Table I of ref. 3 (hereafter referred to as Table I) are reported the effective exponents $k_e = d(\log r)/d(\log t)$, obtained by calculating the slopes between two successive values of $r = \langle r^2(t) \rangle^{1/2}$. To obtain k, the expression $k_e = k + \text{const} \cdot r^{-\alpha}$ was assumed in ref. 3, and the root-mean-square (rms) deviation of the data as a function of α was calculated. The lowest rms deviation occurs at $\alpha \cong 1.0$. Since the data of k_e versus $1/r$ show a curvature for small values of r, only larger values of r were considered and a final linear-least-square fit yielded $k = 0.19 \pm 0.01$. The error 0.01 was estimated from those α's for which the rms deviation differed by a factor of two from its minimum value at $\alpha \cong 1.0$. The data were also analyzed by taking $\alpha = 1$ and fitting k between four successive values of r, and taking k_e as the intercept of this straight-line fit (thus allowing for higher-order corrections). This procedure yielded the k_e values displayed in the fourth column of Table I, and $k = 0.190 \pm 0.001$ was obtained from the last numerical points ($n \geqslant 8$ in Table I). From this new calculation it was concluded that the error 0.01 found above was too large, and the error 0.003 was taken. The value $k = 0.190 \pm 0.003$ thus obtained in ref. 3 is close to the results of ref. 4 and seems to be apparently confirmed by ref. 5. A recent reanalysis of the same data with two correction terms of the form $\text{const}/(\ln t) + \text{const}'/t$,[6] yielded the slightly larger value $k = 0.195 \pm 0.001$. Using $\beta/\nu = 0.4646 \pm 0.0201$,[7] and $\nu = 0.88 \pm 0.02$,[8] in the above equations together with $k = 0.190 \pm 0.003$, one obtains $d_w = 4.041 \pm 0.083$ and $\mu = 2.205 \pm 0.090$.

This value for μ is in conflict with recent calculations of the conductance of finite three-dimensional random resistor lattices, which give $\mu = 2.003 \pm 0.047$,[9] and $\mu = 2.02 \pm 0.04$,[10] and with the series expansion value $\mu = 2.02 \pm 0.05$.[7] Theoretical arguments supporting a value $\mu \cong 2.0$ have been given recently. It has been shown rigorously that for hierarchical node-link-blob models of the conducting backbone, $1 \leqslant \mu \leqslant 2$ for $2 \leqslant d \leqslant 3$.[11] Based on these bounds and the fact that the value $\mu = 2$ is exact for one particular hierarchical model in $d = 3$, it has been conjectured that $\mu = 2$ may be exact for the actual backbone near p_c in three dimensions.[9,11]

Motivated by the inconsistency of the ant-in-the-labyrinth value with the above quoted results,[7,9–11] we have carefully reanalyzed the data of ref. 3, to find out whether the present inconsistency is real or a result of the method of analysis employed. To this end, we have considered different forms for the corrections to scaling and systematically studied their effects on the value of k.

We consider the exponents k_e reported in the third column of Table I, and follow the ansatz

$$k_e = k + \text{const} \cdot t^{-\alpha} \tag{3}$$

According to (3), the natural way of plotting the data to see how good the ansatz actually works is to observe $\ln(k_e - k)$ as a function of $\ln t$. Keeping this idea in mind, we write (3) in the form $\ln(k_e - k) = \ln \text{const} - \alpha \ln t$, which should show a linear dependence of $\ln(k_e - k)$ versus $\ln t$. To proceed further, we take k as a parameter, and obtain ln const and α by a linear least-square fit. The best value of k and its error are, then, estimated by visual inspection of different plots. This procedure has the advantage that one can take into account the magnitude of the estimated error bars, while a weighted least-square fit would only include their relative values. We obtain (see Fig. 1)

$$k = 0.197 \pm 0.004 \tag{4}$$

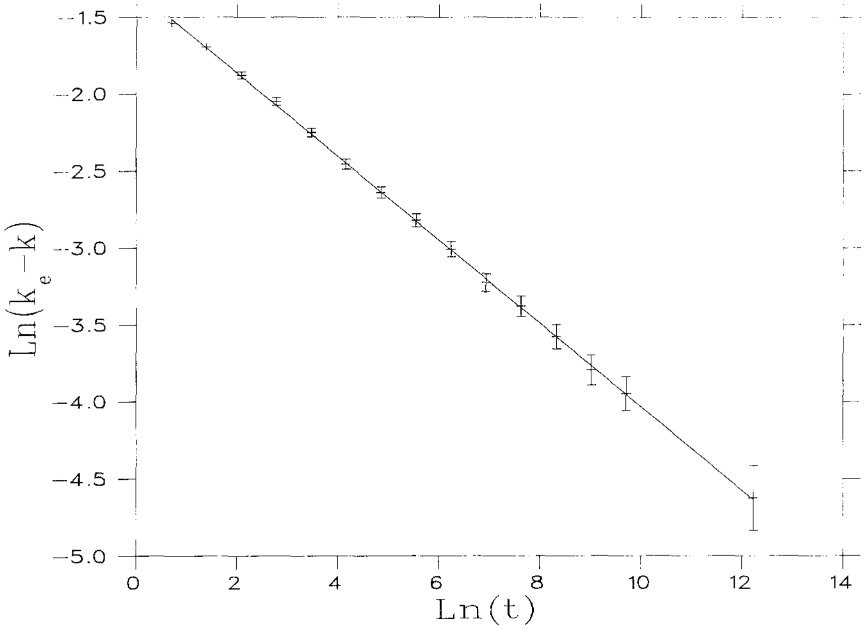

Fig. 1. Plot of $\ln(k_e - k)$ versus $\ln t$ for $k = 0.197$, with k_e from the third column of Table I of ref. 3. The error bars are the estimated 1% statistical error. The straight line is the result of the least-square fit with $\alpha = 0.271 \pm 0.002$ and $\ln(\text{const}) = -1.32 \pm 0.01$; see Eq. (3).

which is larger than the values reported in refs. 3–5, but is not in disagreement with ref. 6. In order to check that the above calculation of k is not biased by us, we have performed a least-square fit with the three parameters in (3) independently, and confirmed our result 0.197. In obtaining (4), we note that the value $k_e = 0.2068$ at $n = 17$ (i.e., $t = 2^n$) in Table I is the average over $15 \leqslant n \leqslant 19$. This value of k_e was used in Eq. (3) in correspondence with the average time $\langle t \rangle = 6.2 \times 2^{15}$ ($\neq 2^{\langle n \rangle}$). According to (4), we obtain the new estimates $d_w = 3.9 \pm 0.1$ and $\mu = 2.08 \pm 0.09$, which are consistent with the results of refs. 7 and 9–11.

We have also analyzed several other possibilities for fitting the data. In all cases we obtain results consistent with (4). Using, for instance, $\langle r^2(t) \rangle = at^{2k} + bt^{\alpha}$, a least-square fit to the second column of Table I yields $k \cong 0.194$, but the least-square fit is satisfactory for larger times only. Indeed, a value $k \cong 0.20$ is consistent with all the data, including the shorter times. The ansatz $r = \langle r^2(t) \rangle^{1/2} = at^k(1 + b/\ln t + c/t)$ (which is similar to the one used in ref. 6) yields $k = 0.200$ ($a = 1.408$, $b = -1.261$, and $c = 2.248$), but again the fit is not good for shorter times. (We mention that $k = 0.195$, $a = 1.508$, $b = -1.261$, and $c = 2.248$ give results similar to the case $k = 0.200$.) Using the successive slopes values k_e again, we find for the ansatz $k_e = k + a/\ln r + b/r$ the result $k = 0.195$, with $a = -0.013$ and $b = 0.240$; however, the fit does not work well for smaller r. These results indicate that if correction terms of the form discussed in this paragraph are introduced, more free parameters are needed to get a satisfactory fit of the data at smaller r. However, too many fitting parameters are not recommended, since with a sufficient number of parameters almost any value of k can be fitted. We have still considered the five-parameter form $k_e = k + a/r^{\alpha} + b/r^{\beta}$, and a least-square fit to the data yielded $k = 0.193 \pm 0.004$, with $a = 0.734$, $b = -0.550$, $\alpha = 1.309$, and $\beta = 1.520$.

The result (4) may also be tested in a different way, by calculating the fitting parameter k in (3) as a function of the upper time t_N, where the data for $t > t_N$ is excluded from the fit. Following this procedure, a least-square fit of the three parameters in (3) yields the values $k(t_N) = 0.197$, 0.196, 0.195, 0.195, 0.194, 0.191, and 0.190, with $\alpha = 0.272$, 0.267, 0.263, 0.265, 0.261, 0.249, and 0.249, for $t_N = 6.2 \times 2^{15}$, 2^{14}, 2^{13}, 2^{12}, 2^{11}, 2^{10}, and 2^{9}, respectively. This calculation suggests that the actual value of k in (1a) is possibly larger than (4).

A further test to (4) is considering "second-order corrections" to the expression (3) directly. Since the appropriate way to test the ansatz (3) is observing $\ln(k_e - k)$ as a function of $\ln t$, it seems to us that a term $\sim (\ln t)^2$ should be the natural choice for introducing another correction term. Thus, we propose to rewrite (3) in the new more general form

$$\ln(k_e - k) = \ln \text{const} - \alpha \ln t - \alpha'(\ln t)^2 \tag{5}$$

with four unknown parameters instead of three as in (3). Taking k as a parameter, we obtained ln const, α, and α' by a least-square fit. By a visual inspection of different plots, confirmed by a full least-square fit of the four parameters in (5), we obtain now $k = 0.200 \pm 0.002$, with $\ln \text{const} = -1.37 \pm 0.02$, $\alpha = 0.251 \pm 0.005$, and $\alpha' = 0.0038 \pm 0.0004$, supporting our result (4) and the suggestion $k \geqslant 0.197$. Note that the "second-order correction" term in (5) increases more rapidly with time than the first-order one, in contrast to the usual behavior assumed for the above discussed more standard forms, in which higher correction terms vanish more rapidly than the lower order terms. This does not mean, however, that (5) is unrealistic for larger times. Indeed, (5) implies that $k_e = k + \text{const} \cdot t^{-(\alpha + \alpha' \ln t)}$, thus $k_e \to k$ for $t \to \infty$, and there is no *a priori* reason for expecting the $(\ln t)^2$ term in (5) to remain always smaller than the first-order term. We will see at the end of this paragraph why we still call it a second-order term. This unusual behavior indicates that the correction terms may be playing a more important role than normally expected. Due to the slow convergence of the correction terms in (5), it follows that the numerical points obtained for shorter times cannot be neglected. For the present data, we find that $\alpha' \ll \alpha$, indicating that the second correction term remains small compared with the first correction term, even for the largest available time $t = 6.2 \times 2^{15}$. This is consistent with the results shown in Fig. 1, where within the estimated statistical errors no clear systematic deviation of the points is observed, and "second-order corrections" to (3) are expected to be small.

When the correction term is a function of r, instead of t as in Eq. (3), the ansatz $k_e = k + \text{const} \cdot r^{-\alpha}$ was again applied, but no satisfactory result was obtained, indicating that higher order corrections are clearly required in this case. Here, we implement such a procedure by replacing $\ln t$ by $\ln r$ in (5). The best fit yields $k = 0.200 \pm 0.002$ ($\ln \text{const} = -1.74 \pm 0.02$, $\alpha = 0.68 \pm 0.03$, and $\alpha' = 0.21 \pm 0.01$), in remarkable agreement with the result obtained from (5), where now α and α' are of the same order of magnitude. The value $k = 0.200 \pm 0.002$ is in disagreement with refs. 3–6.

Although the same value $k \cong 0.200$ is obtained as a function of $\ln t$ and of $\ln r$ with second-order corrections according to the scheme (5), we take as our more conservative estimate the value $k = 0.197 \pm 0.004$, obtained with the simpler ansatz (3). This estimate includes all the previously discussed values of k obtained with different ansatz and the results of ref. 6, and is still consistent with ref. 3 within the error bars.

CASE (b)

Let us discuss now the evaluation of the second exponent d_w, obtained in ref. 3 using the exact enumeration technique[1] for systems of up to 120^3 sites; there it was found that $d_w = 4.00 \pm 0.05$ using the ansatz $1/d_{we} = 1/d_w + \text{const} \cdot r^{-\alpha}$. Here, we apply the approach $1/d_{we} = 1/d_w + \text{const} \cdot t^{-\alpha}$ to the same data, the sixth column of Table I, following the same method discussed previously for the ansatz (3). We obtain $d_w = 4.05 \pm 0.22$, consistent with the results of ref. 3, but with larger error bars, indicating an underestimation of the errors in ref. 3. This value is also consistent with the result $d_w = 3.9 \pm 0.1$ calculated using (4). When the parameters $d_w(t_N)$ are calculated from fits excluding times $t > t_N$, as similarly done for obtaining $k(t_N)$, we find that $d_w(t_N)$ is a decreasing function of t_N, indicating that $d_w < 4.00$. Further computational work, for larger systems and times t, is required to improve the numerical results in this case.

As discussed in ref. 1, the actual value for d_w is bounded by

$$d_f + 1/\nu \leqslant d_w \leqslant d_f + d_f/d_l \tag{6}$$

where $d_f = d - \beta/\nu$ is the fractal dimension and $d_l = \tilde{\nu} d_f$ is the chemical dimension.[1] Accurate values for $\tilde{\nu}$ have been obtained recently in three dimensions, $1/\tilde{\nu} = 1.34 \pm 0.01$.[12] Using $\beta/\nu = 0.4646 \pm 0.0201$,[7] and $\nu = 0.88 \pm 0.02$,[8] in Eq. (6), we find

$$3.672 \pm 0.046 \leqslant d_w \leqslant 3.875 \pm 0.022 \tag{7}$$

Our result $d_w = 3.9 \pm 0.1$ is in agreement with these bounds. It should be emphasized that the Alexander–Orbach rule,[13] $d_w = 3d_f/2 = 3.80 \pm 0.03$, is consistent with the presently available numerical results.

In summary, it becomes clear that more theoretical work is needed in order to assert the correct dependence of the correction to scaling terms. Until this is available, it is important to find simple correction terms that enable one to simultaneously fit the whole set of data. In other words, the corrections to scaling should be as simple as possible compatible with *all* the numerical points. To omit some of them in any stage of the analysis may conduce to incorrect results.[3] We have found that these correction terms show a slower convergence of the effective exponents $k_e \to k$ than would be usually expected. The more involved corrections proposed in ref. 6 to analyze the same data do not provide, at small r, satisfactory fits. The simpler ansatz $k_e = k + \text{const} \cdot t^{-\alpha}$ gives, within the statistical error bars, a rather satisfactory fit of the data with $k = 0.197 \pm 0.004$ ($d_w = 3.9 \pm 0.1$). When another correction term is included, Eq. (5) is found to be the most satisfactory one, and $k \cong 0.20$ is obtained, supporting the first-order result. Both values are consistent with the results of refs. 7, 9, and 10, and with the bounds in Eq. (7).

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