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Short Communication

Diffusion in Three-Dimensional Random Systems at Their Percolation Thresholds

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Extensive Monte Carlo simulations of the *ant-in-the-labyrinth* problem on random $L * L * L$ simple cubic lattices are performed, for L up to 960 on a CRAY-YMP supercomputer. The exponent k for the rms displacement r with t in $r \sim t^k$ is found to be $k = 0.190 \pm 0.003$. As a second approach, large percolation clusters with chemical shells up to 300 are generated on a simple cubic lattice at criticality. The diffusion equation is then solved by using the exact enumeration technique. The corresponding critical exponent d_w is found to be $1/d_w = 0.250 \pm 0.003$.

KEY WORDS: Percolation; anomalous diffusion; Alexander–Orbach rule; vector computer.

Diffusion in random percolating systems, known as the *ant-in-the-labyrinth* problem after de Gennes,[1] has attracted much attention in the recent years. According to the usual scaling theory of percolation,[2] the description of such dynamical aspects as, e.g., the conductivity ($\sim$ diffusion constant) in random resistors networks requires the knowledge of a dynamic critical exponent, which, in general, *cannot* be related exactly to the static critical exponents.

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Alexander and Orbach[3] made the interesting observation, based on empirical data, that a certain combination of static and dynamic exponents (see below), called the fracton or spectral dimension, is about 4/3 for dimensions $d > 1$. In order to test this conjecture, extensive numerical and analytical work was initiated. High-accuracy Monte Carlo simulations found deviations by 2–3% for two dimensions,[4] whereas series expansions[5] were consistent with the AO rule. In high dimensions, it violates an ε expansion[6] around $d = 6$. For the physically most relevant dimensionality $d = 3$, however, the situation is more controversial. While previous Monte Carlo studies gave results in agreement with the AO rule,[7] with a possible exception of ref. 8, in a more recent numerical work an appreciable deviation from this rule was found.[9] In that work, large systems of up to 456^3 sites were considered.

In this work, we attempt once more to improve the numerical accuracy of the Monte Carlo simulations by studying much larger systems (up to 960^3 sites), thus reducing considerably the finite-size effects. We consider two different methods: The first one is the ant-in-the-labyrinth method, i.e., the diffusion of noninteracting particles on the occupied sites of a random simple cubic lattice of linear length L at the percolation threshold $p_c = 0.3116$ (averaged over all cluster sizes). For each of the 100–500 lattices, we used 500–10000 random walkers (ants) and averaged over all of them, independently of whether they started on the infinite percolation cluster or on a finite cluster. In this case the rms displacement r becomes anomalous[10] at the percolation threshold and scales with time t asymptotically as

$$r \sim t^k \tag{1a}$$

The exponent k can be written in terms of static and dynamic critical exponents as

$$2k = (2 - \beta/\nu)/(2 + (\mu - \beta)/\nu] \tag{1b}$$

where ν is the correlation length exponent, β the exponent for the volume fraction of the infinite network, and μ the conductivity exponent.[2] The fracton or spectral dimension d_s of the incipient infinite cluster is related to the exponent k via

$$4k = d_s(2 - \beta/\nu)/(d - \beta/\nu) \tag{1c}$$

Alexander and Orbach[3] conjectured that $d_s = 4/3$ in all dimensions $d > 1$, i.e., it is superuniversal. If this rule holds, then k in (1c) is given simply by

$$3k = (2 - \beta/\nu)/(d - \beta/\nu) \tag{1d}$$

The second method uses the exact enumeration technique,[10] with which we study diffusion on the incipient infinite percolation cluster alone. Thus we generate a large percolation cluster at the critical concentration p_c using the Leath algorithm[11] and solve the diffusion equation by exact enumeration. This is equivalent to an average over *all* possible random walks. Finally, a configurational average over 2000 cluster realizations is performed. In the exact enumeration method one calculates the probability $P(i, t)$ of the walker to be at site i at time t, by knowing the probability to be at site i and at each of its nearest-neighbor sites at time $t-1$. In our case the required transition probabilities to make a time step are just one or zero, depending on whether the neighbor site belongs to the cluster or not, respectively, and are appropriately normalized. In both methods we use the diffusion rule, commonly known as the blind-ant rule, in which the walker has a finite probability to remain in its site i at time t.

Diffusion on the incipient infinite percolation cluster is anomalous[10] such that the rms displacement r behaves asymptotically with time t as

$$r \sim t^{1/d_w} \tag{2a}$$

where the exponent d_w is the so-called fractal dimension of the random walk and is given by

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

Using (1b) and (2b), we can relate d_w to k as

$$d_w k = 1 - \beta/2\nu \cong 0.76 \tag{2c}$$

which provides us with a consistency relation between the two exponents to be measured independently in the simulations. Again, if the AO rule holds, one has

$$d_w = 3(d - \beta/\nu)/2 \tag{2d}$$

Both methods were implemented on the CRAY-YMP at the Höchstleistungs-Rechenzentrum of the KFA at Jülich. The two problems can be vectorized using standard FORTRAN language; no assembler statements as in refs. 7 and 9 were needed. For the first method, in order to simulate large systems we stored each site in one bit and to speed up the algorithm we stored the three-particle coordinates on a single 64-bit word. With the latter improvement about 20% of computing time was saved. We needed about 0.29 μsec/step per ant, which is a bit higher than the 0.22 μsec/step per ant obtained on the CDC Cyber 205 in a previous work.[9] This speed, however, remained constant, in contrast to the perfor-

mance drop observed on the Cyber 205 for larger system sizes.[9] For the lattice occupation we needed about 0.05 μsec/site (compared with 0.06 μsec/site on a Cyber 205). To reach sizes of $L = 960$, a 15-Mword storage was required. The whole lattice was stored on a one-dimensional array, and the same boundary conditions as described in ref. 7 were used. For the second method, the Leath algorithm was not vectorized and required about 0.6 μsec/site. To grow a cluster for which the last grown sites have reached a chemical distance[10] $l = 300$, we used 16-Mword storage for a lattice of 240^3 sites in which each site occupied a single 64-bit word. We could create clusters containing up to 90,000 sites and we checked that they never touched the boundaries. The later exact enumeration, however, where most of the computer time was spent, was more efficient and reached about 100 Mflops/sec, or 0.19 μsec/step, faster than the ant-in-the-labyrinth method. For each method about 22h of CPU time was used.

Let us discuss our results for the first method. We simulated systems with linear sizes $L = 192$, 448, 704, 768, and 960. Usually we considered walks up to 2^{14} time steps and averaged over typically 5×10^5 ants on all independent lattices together. We observed no clear manifestation of finite-size effects, even for $L = 192$, within that time interval. For $L = 704$ and 960, we went up to 2^{19}, with averages over a total number of ants of about 10^5. Again, no apparent finite-size effects as found in ref. 7 were observed, but for $L = 192$ and 448 we again found the effective exponent k_e (see below) to increase for long times. For the most accurate data we restricted the walks to 2^{14} steps and averaged over 3.5×10^6 ants in total. Most of the data were obtained for $L = 960$ (1.6×10^6 ants) and 704 (10^6 ants). As in previous works,[7,9] our aim is to find the asymptotic exponent k in (1a). In Table I we report the averaged values of $r(t)$ for times $t = 2^n$, with $0 \leqslant n \leqslant 14$. The value for $n = 17$ is a linear least-square fit of the data of $r(t)$ for $15 \leqslant n \leqslant 19$, obtained with less accuracy for $L = 960$ and 704. In the third column of Table I we include the effective exponents $k_e = d(\log r)/d(\log t)$, obtained by calculating the slopes between two successive values of r. The data of k_e versus $1/r$ are very similar to the results shown in Fig. 1 of ref. 9, and therefore are not plotted here again. Since the data of k_e versus $1/r$ show indeed a curvature for smaller r, we assumed $k_e = k + \text{const} \cdot r^{-\omega}$ and calculated the root-mean-square deviations as a function of ω (a plot of k_e versus $1/\log t$ showed a much pronounced curvature and was not included in the analysis). This procedure was repeated by successively omitting data for n smaller than a given n_c. We obtained stable results (independent of n_c) for $7 \leqslant n_c \leqslant 11$. In this interval, the lowest rms deviation occurred at $\omega_m \cong 1.0$, which corresponds to $k \cong 0.19$. The error bars for k are obtained from those values of ω for which the rms deviation

differs by a factor of two from its minimum value at ω_m. This gives $k = 0.19 \pm 0.01$. Since this calculation may overestimate the error bars, we analyzed the data in a different way. We calculated new k_e exponents from those given in Table I by a linear least-square fit between four successive values, r_{n+3}, r_{n+2}, r_{n+1}, and r_n. The corresponding intercept of the straight line at $1/r = 0$ was taken as the new value for k_e at r_{n+1}. These are reported in the fourth column of Table I. We observe a constant value 0.190 ± 0.001 over a large interval of distances. This result provides us with a much lower error estimate than found above. Thus, for a more realistic estimate we take the geometric average of the two error bars, which leads to

$$k = 0.190 \pm 0.003 \tag{3}$$

Table I. Averaged RMS Displacements Traveled by the Diffusing Ants and Effective Exponents k_e for Times $t = 2^n$ [a]

n	r	k_e	k_e	r	$1/d_{we}$	$1/d_{we}$
0	0.5582	—	—	0.6203	—	—
1	0.7427	0.4122	—	0.8289	0.4181	—
2	0.9670	0.3807	0.2488	1.0885	0.3932	0.2972
3	1.2326	0.3500	0.2251	1.4077	0.3709	0.2822
4	1.5449	0.3258	0.2087	1.7961	0.3516	0.2714
5	1.9051	0.3024	0.1970	2.2646	0.3344	0.2646
6	2.3177	0.2828	0.1954	2.8276	0.3204	0.2604
7	2.7915	0.2684	0.1953	3.5030	0.3090	0.2562
8	3.3347	0.2565	0.1907	4.3095	0.2989	0.2528
9	3.9558	0.2464	0.1903	5.2703	0.2904	0.2509
10	4.6615	0.2368	0.1906	6.4142	0.2833	0.2506
11	5.4712	0.2311	0.1909	7.7744	0.2775	
12.	6.3944	0.2250	0.1899	9.3937	0.2729	
13	7.4452	0.2195	0.1901			
14	8.6492	0.2163				
15	10.001	—				
16	11.558	—				
17	13.247	0.2068				
18	15.392	—				
19	17.745	—				

[a] The k_e were obtained by calculating the slopes between two successive values r_{n-1} and r_n. The value for $n = 17$ is an average over $15 \leqslant n \leqslant 19$. The fourth column contains values of k_e obtained as intercepts of straight lines fitted through four successive r values. The fifth and sixth columns display averaged rms displacements obtained by exact enumeration and effective exponents $1/d_{we}$, for times $t = 2^n$, respectively. The exponents $1/d_{we}$ were obtained by calculating the slopes between two successive values r_{n-1} and r_n. The seventh column contains values of $1/d_{we}$ calculated as done for k_e in the fourth column. The error bars for k_e and $1/d_{we}$ in columns three and six, respectively, are about ± 0.003.

We can now compare this result with that expected from the AO rule (1d). Using accurate values[12] for the ratio $\beta/\nu \cong 0.477$, we find $k_{AO} = 0.201 \pm 0.001$. Clearly, our value (3) appears to be barely inconsistent with this AO rule. Using (1b), we deduce a new value for the ratio $\mu/\nu = (k^{-1} - 2)(1 - \beta/2\nu) = 2.48 \pm 0.07$, slightly inconsistent with the recent[13] series value 2.31 ± 0.06. Finally, using (2c), we deduce $d_w = 4.0 \pm 0.07$, which we proceed to test independently as shown next.

Using the Leath algorithm,[11] we generated large percolation clusters on the simple cubic lattice at criticality. Clusters which have not reached a given chemical distance l were rejected, while the growth was stopped when they reached l. In order to get some estimate for possible finite-size effects, we studied separately clusters for $l = 100$, 200, and 300. The diffusion equation was solved with the exact enumeration technique[10] for up to 2^{12} time steps with averages over 2000 different clusters for each value of l. We are interested in the asymptotic value of the exponent d_w defined in (2a). Following the same procedure discussed above for the first method, we calculated the effective slopes d_{we} from the measured rms displacements $r(t)$. These results are given in the fifth and sixth columns of Table I, which contain averages of the rms displacements over the three system sizes l. By calculating separately the effective exponents d_{we} obtained for each l, we observed indeed no systematic deviation between the data which could be attributed to finite-size effects. Since again a curvature is observed in the final data of $1/d_{we}$ versus $1/r$, a linear least-square fit of the data was performed. Here we assume $1/d_{we} = 1/d_w + \text{const} \cdot r^{-\omega}$ and apply the same procedure discussed above for the first method. In this case, however, the fit is not successful since a plateau is not obtained as in the first method. A linear least-square fit for $n \geqslant 8$ gives $1/d_w = 0.251 \pm 0.009$. To check the stability of this result, we reanalyzed the data by calculating the effective intercepts $1/d_{we}$ between four successive r values as described above for obtaining k_e in the fourth column of Table I. The new effective exponents are reported in the seventh column of Table I. They seem to approach a straight line for $n \geqslant 9$ and extraplate to 0.250 ± 0.001, close to the above value. Again, as error bars we take the geometric mean, which gives $1/d_w = 0.250 \pm 0.003$ or

$$d_w = 4.00 \pm 0.05 \tag{4}$$

consistent with (3) through (2c). We can compare this value from that expected from the AO rule (2d), which gives $d_{wAO} = 3.785 \pm 0.01$. We find a clear disagreement between this and our value (4). From series results[13] we deduce a value for $d_w = 3.83 \pm 0.06$ barely consistent with our result (4). We can estimate again a value for the ratio μ/ν using (2b) and (4). We find in excellent agreement with the first method, $\mu/\nu = 2.45 \pm 0.05$, which is

again slightly larger than the series[13] value 2.31 ± 0.06. It is worthwhile to mention that much information is contained in the probability density $P(r, t)$, obtained as a by-product of the exact enumeration method, which we have not discussed here. This function gives the probability to find the random walker at time t at a distance r from its starting point. Of current interest is the study of the fluctuations of $P(r, t)$ for fixed r and t through the averaged moments $\langle P^q(r, t) \rangle$ for any real $q > 0$, as was recently done for percolation in two dimensions.[14] A similar study in three dimensions will be reported elsewhere.

In summary, we have attempted to improve the numerical accuracy of the existing Monte Carlo data for the anomalous diffusion exponent k of the ant-in-labyrinth problem in three dimensions. This is accomplished by studying much larger systems (up to 960^3 sites) than in previous works. Our estimate for $k = 0.190 \pm 0.003$ appears barely inconsistent with the Alexander–Orbach rule $k = 0.201 \pm 0.001$, while our value lies between the previous 0.20 ± 0.01 obtained in ref. 7 and 0.175 ± 0.01 in ref. 9. Independently of the above method, we studied diffusion on the incipient infinite percolation cluster and solved the diffusion equation by exact enumeration. We studied clusters containing up to 300 chemical shells. We obtain $d_w = 4.00 \pm 0.05$ (or $1/d_w = 0.250 \pm 0.003$) for the corresponding anomalous diffusion exponent, which deviates somewhat from the AO rule, $d_w = 3.785 \pm 0.01$. This work is possibly the first attempt to implement the exact enumeration technique on a 64-bit word vector computer, and clearly future work in this direction should be encouraged. The slight deviation from the AO rule in three dimensions complements that found in two dimensions[4]; it contradicts somewhat the series results for two and three dimensions,[13] which agree with the AO rule. This discrepancy remains to be understood.

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