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Monte Carlo Evidence for the Deviation from the Alexander–Orbach Rule in Three-Dimensional Percolation

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Computer simulation is used to study the diffusion at the percolation threshold on large simple cubic lattices. The exponent k for the rms displacement r with t in $r \sim t^k$ is found to be smaller than 0.2, while the Alexander–Orbach 4/3 rule for the spectral dimension predicts $k = 0.201 \pm 0.002$.

KEY WORDS: Percolation; diffusion; vector computer; Alexander–Orbach rule; and in the labyrinth.

The usual scaling theory of percolation[1] relies on two critical exponents for the static properties, while the dynamic aspects, such as the conductivity of random resistor networks, require a third exponent. Alexander and Orbach[2] found empirically that a certain combination of these three exponents (see below), called the fracton or spectral dimension, is about 4/3. Later, high-accuracy Monte Carlo simulations found deviations by 2–3% for two dimensions,[3] whereas series expansions[4] were consistent with this AO rule. In high dimensions the so-called epsilon expansion[5] disagrees with the AO rule. However, for the physically most relevant dimensionality $d = 3$ most data, with a possible exception of Ref. 6, are consistent with the AO rule. Here we attempt once again to increase the accuracy of the Monte Carlo simulation to test the validity of the AO rule.

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We use the ant in the labyrinth method, i.e., the diffusion of non-interacting particles on the occupied sites at the percolation threshold (average over all cluster sizes). For every lattice we used many walkers and averaged over all of them, whether they started on the infinite network or on a finite cluster. In this case the asymptotic power law for the rms displacement r at time t becomes anomalous at the percolation threshold[11,1,7]:

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

$$k = 2(2+\vartheta)/D \tag{1b}$$

$$\vartheta = (\mu - \beta)/\nu \tag{1c}$$

$$D = d - \beta/\nu \tag{1d}$$

where ν is the correlation length exponent, β the exponent for the volume fraction of the infinite network, μ the conductivity exponent, and D the fractal dimension. The fracton or spectral dimension $\bar{d}$ or d_s of the incipient infinite cluster is related to the exponent k via

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

Alexander and Orbach[2] conjectured that d_s is superuniversal, i.e., it equals 4/3 in all dimensions $d > 1$.

The implementation of this problem on the CDC Cyber 205 at Bochum University was described in detail in Ref. 7 and is used here again. However, that work was strongly hampered by finite-size effects even though lattices of size $L * L * L$ with L up to 256 were used. In the meantime, the main memory of the Bochum installation was increased from one-half megaword to two megawords of memory, and thus simulations with larger lattice sizes with L up to 456 were possible. Since the diffusion time t scales with a rather large power of length (see Ref. 1 or 7 for a review of the scaling theory), such a small increase in length scale L shifts the diffusion time (where finite-size effects become visible) by a large amount.

The parameters regarding the statistics and implementation of the method are described as follows. We use 20 independent lattices each up to 2 ** 19 time steps with $L = 456$, and 1500 independent lattices each up to 2 **15 time steps with $L = 376$ on the expanded Bochum machine. On each lattice, 512 ants were allowed to diffuse randomly. For each step per ant, apart from the initialization, we needed about 0.22 μsec for $L = 176$, 256, 360, and 376. The time increased to 0.46 μsec for $L = 416$ and to even 0.73 μsec for $L = 456$. Therefore our best data were restricted to $L = 376$. Our main aim is to find the asymptotic exponent k for $r \sim t^k$. Figure 1 shows the results, plotted[7] as effective exponent $k_e = d(\log r)/d(\log t)$ versus $1/r$. The results of Ref. 7 are also shown for comparison.

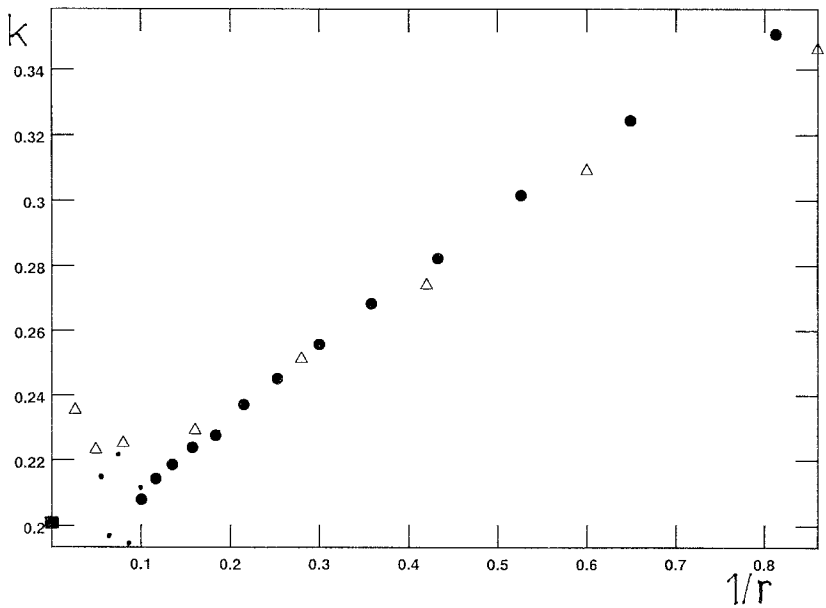

Fig. 1. Effective exponent k versus reciprocal rms distance traveled by the diffusing ants. Large circles refer to $L=376$ with good statistics, dots to $L=456$ with bad statistics and longer runs. The triangles gives the results from Ref. 7 for $L=256$. The solid square indicates the Alexander–Orbach conjecture $k=0.20$.

We see that the finite-size effects in Ref. 7 (the upturn for the largest times and distances) gave a misleading impression that the data follow a straight line in an intermediate time region. Thus, Ref. 7 concluded $k=0.20\pm0.01$. Our present data show some curvature in the opposite direction and we therefore extrapolate by making the ansatz $t\sim r^{1/k}(1+\text{const}\cdot r^{-\omega})$. Figure 2 shows the sum of the squared deviations from the good data points (run with 1500 lattices only) and suggests

$$k=0.175\pm0.01 \tag{3}$$

This estimate is based on fits of data for large r, excluding small distances r. Our data give the best fit with ω near 0.8. Data in Fig. 1 for the larger systems suggest that finite-size effects are quite small now. Our k and the conductivity exponent μ are related by $\mu/\nu=(k^{-1}-2)(1-\beta/2\nu)=2.8$, where ν is the correlation length exponent. This estimate 2.8 ± 0.3 is appreciably higher than previous values near 2.3, as cited in Ref. 7. Our correction ansatz may be too simple, which means that higher order corrections to scaling in r versus t are needed for a reliable quantitative estimate. Right now, the visual impression from Fig. 1 may be quite naive,

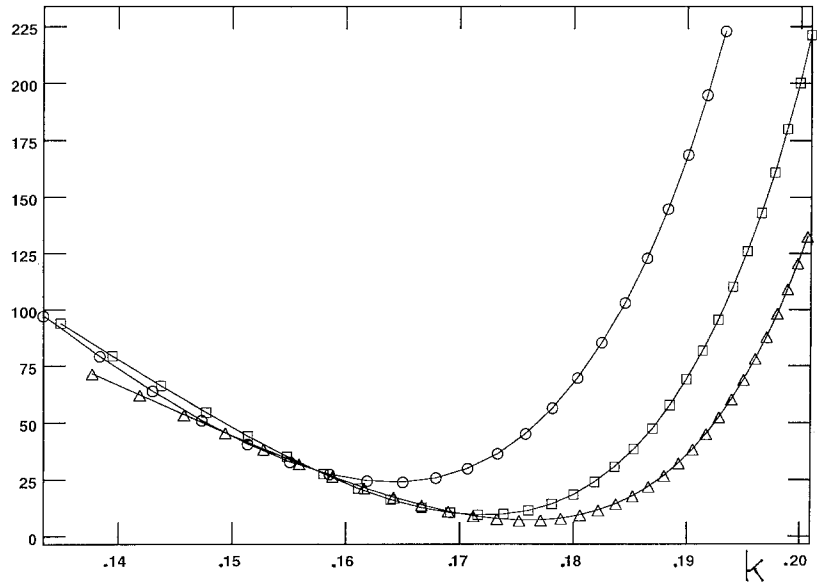

Fig. 2. Mean square deviation (arbitrary units) of measured effective exponents k_e from the fit $k_e = k + \text{const} \cdot r^{-\omega}$, versus fitted k. Here ω varied between 0.5 and 1.1. Data for times below 4, 8, and 16 were omitted in the fits symbolized by circles, squares, and triangles. If even longer times are omitted, the minima stay near $k = 0.175$, but become flatter.

but may be the best choice. Direct inspection of these data indicates that they are very difficult to reconcile with $k = 0.20$. The Alexander–Orbach rule in d dimensions predicts[7]

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

where β is the critical exponent for the order parameter. From the series expansion[8] result, $\beta/\nu = 0.49 \pm 0.04$, which gives $k = 0.201 \pm 0.002$, in contradiction to the numerical result (1). We simulated this diffusion process at the percolation threshold of 0.3116 from Ref. 9. Runs at different concentrations suggest that the inaccuracy of about 0.0002 in the threshold gives an error in k smaller than our statistical error.

It has to be explained why the Cyber 205 CPU performance drops by a factor of three on increasing the system size beyond 376. Total storage requirement for the three-dimensional lattice, using one bit per site, is $(L+42) * L * L/2 ** 22$ large pages, where a large page is 65536 64-bit words, the unit of storage on the Cyber 205. System size $L = 376$ corresponds to the limit of 15 large pages total storage. The physical main memory size available at the Bochum installation is greater than 25 large

pages. Therefore, page thrashing to/from the mechanical disk drives cannot be the problem.

The Cyber 205 is a virtual memory machine, that is, the memory addresses in user's programs do not point to physical memory locations, but rather to virtual ones. A translation mechanism is required to obtain physical memory address from virtual memory address. This translation mechanism is provided by the page table: for each page allocated to the user, the virtual address of the first word within that page is related to a physical address in memory. All other words within the same page may then be found by adding suitable address offsets.

If a program is using 25 large pages, it obviously has to have a 25-element page table giving the actual memory locations for the 25 pages. Since the memory access is performed by the gather instruction exclusively for the present algorithms, each and every random sequence of 25 table elements is accessed with equal probability. Unfortunately, in Cyber 205 there is only a set of 16 hardware associative registers to hold the 16 most recently used page table elements. If in the course of the gather instruction a page outside the last set of 16 pages is accessed, i.e., its page table element is required, this element will not be found in the hardware associative registers. In this case the vector gather instruction will be interrupted, and the hardware associative registers will be reloaded from the central memory with new elements of the page table and will again be searched for the required element. Because the sequence of page table elements required is random, it is obvious that this interruption will occur with a probability equal to (total number of pages -16)/(total number of pages). The total number of pages is one larger than the number of data pages because one page is needed to hold the program code, local and auxiliary variables, and the like. Therefore, up to 15 data pages, the vector gather instruction will not be interrupted and will exhibit maximum performance. For larger and larger systems, the above probability will tend to one, that is, the gather instruction will be interrupted for each element, leading to much longer execution times, as we observed in this simulation (see above).

In summary, we have shown that the memory of a fast computer should be commensurate with its speed. With the bigger memory we could obtain better results with about the same computer time than that of Ref. 7. We found a deviation from the Alexander–Orbach rule for three-dimensional percolation. The corrections to scaling are possibly nonlinear, $\omega < 1$, or more than one correction term is needed for these data. It would be nice to confirm this result by other techniques, for example, the exact enumeration[10] of occupation probabilities for a given randomly constructed lattice.

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