Diffusion of Lattice Gases without Double Occupancy on Three-Dimensional Percolation Lattices

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We examined the diffusion of lattice gases, where double occupancy of sites is excluded, on three-dimensional percolation lattices at the percolation threshold p_c. The critical exponent for the root-mean-square displacement was determined to be $k = 0.183 \pm 0.010$, which is similiar to the result of Roman for the problem of the "ant in the labyrinth." Furthermore, we found a plateau value for k at intermediate times for systems with higher concentrations of lattice gas particles.

In recent last years much effort has gone into the study of disordered systems. One of the simpler aspects of disorder is described with percolation theory.[1] Transport of particles on lattices with randomly blocked sites is of interest, e.g., for random resistor networks. To study such transport phenomena, particle diffusion on percolation lattices is investigated.

Particularly at the percolation threshold p_c the behavior of the root-mean-square displacement

$$R = \langle R^2 \rangle^{1/2} \propto t^k \tag{1}$$

should be universal, i.e., the critical exponent k should be equal for different diffusion mechanisms on a percolation lattice, if only the disorder rules the diffusion processes.

The investigation of Eq. (1) was stimulated by the *ant in the labyrinth* problem of de Gennes.[2] Study of such random walkers on percolation lattices has been the topic of many publications.[3–17] For three-dimensional

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systems the value of the critical exponent is still not precisely known. The most accurate value was obtained by Roman[17] as $k = 0.190 \pm 0.003$. This value differs from the hypothesis of Alexander and Orbach,[3] $k = 0.201$.

The above-mentioned investigations were restricted to single-particle diffusion, or in other words to the noninteracting case. A lattice gas without double occupancy of sites is one of the next most complicated models. In this model, one may distinguish between collective and tagged-particle diffusion.[18] Here we are concerned with the tagged-particle or tracer diffusion. Both models, the ant in the labyrinth and the lattice gas, might belong to the same universality class, and then their critical exponents should be equal. Therefore, simulations of a lattice gas without double occupancy on percolation lattices were made above, below, and at the percolation threshold p_c.[19–23] The static properties of percolation effects of lattice gases were examined recently.[24] Heupel determined the critical exponent k at the percolation threshold as $k = 0.199$, in agreement with the early result of Pandey et al.,[13] but no error bars were given. Further a finite-size effect, similar to the results of ref. 13, was detected, where the exponent k increases for longer times of the simulation. The results were determined for relatively small lattices and very low concentrations of the lattice gases, because of the restricted resources of computer time and storage on the CDC Cyber 76. At this time the standard algorithm for simulations on this model[25] was not vectorized. Recently, a fully vectorizable algorithm for simulations of lattice gases without double occupancy of sites was developed.[26] Using this algorithm we reexamined the problem of such a lattice gas on a three-dimensional percolation lattice at $p_c = 0.3116$. The aim of this work is to calculate more accurately the critical exponent k for larger lattices and higher concentrations of diffusing particles.

The update rate decreases in this application of the algorithm to a value of 1–2 μsec per update, depending on the concentration. This is a factor of two to four slower than on the regular lattice[26] with a concentration of 50 %. This decrease is not unexpected, because the simulations were done at a very low concentrations and nearly 70 % of all sites were forbidden. Therefore the vector length of the sublattices decreases to values around 250 or even shorter. On the CRAY X-MP/416, where these simulations were performed, the highest performance is available at vectorlength 64 or multiples of this value. For very long vectors the loading time of the 64-element vector register can be neglected compared to the gain in speed. But for vector lengths we used, this is not the case. This causes a decrease in the update rate. If one uses another sublattice structure with less sublattices as proposed in ref. 26, the update rate could be increased significantly.

To determine k, we analyzed our data for a particle concentration of

10% of the allowed sites, which is a concentration of 3.116% relative to the size of the whole lattice. During the simulation we calculated the mean-square displacement at times t, which were a power of 2. The longest investigated time was 2^{15} Monte Carlo steps. After the end of the simulation we calculated the root-mean-square displacement. We determined the exponent k at each time by

$$k = \frac{d \log R}{d \log t} \tag{2}$$

Then we took three or more consecutive values for k and fitted them onto a straight line in a plot versus $1/R$. From the resulting intercept we calculated the asymptotic value of k for $R \to \infty$.

We estimated the asymptotic exponent $k = 0.181 \pm 0.010$ for a system of size 30^3 and 1000 lattices. For systems with $L = 60$, we did simulations on 70 lattices with similar accuracy and got the plot of Fig. 1. The straight lines are fits to certain sets of data. For times 2^{13} to 2^{15} and 2^{10} to 2^{12}, linear fits gave an asymptotic exponent of $k = 0.175$. A linear fit through all these points gave an exponent of $k = 0.183$. For intermediate times the asymptotic exponent was evaluated to be $k = 0.206$. All these values have
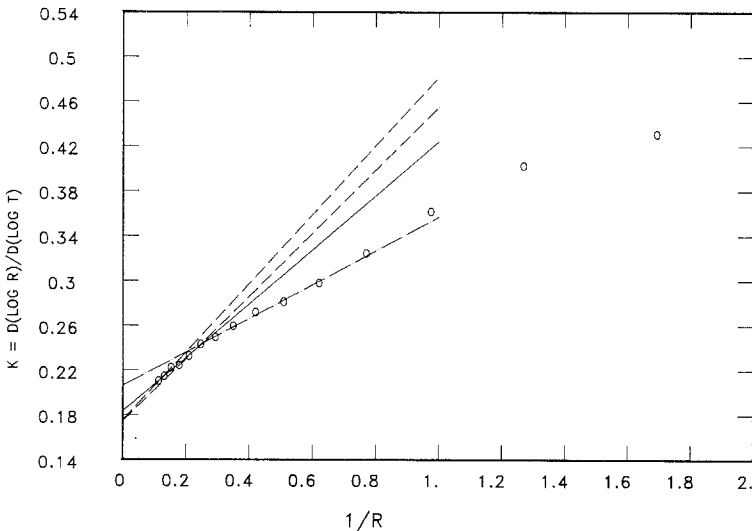

Fig. 1.   The exponent k versus $1/R$ for lattices gases on three-dimensional percolation lattices at the percolation threshold with $L = 60$. Circles are simulation data. The dashed-dotted lines are linear fits through the data for the exponents $n = 13$–15 and $n = 10 - 12$ of the time $t = 2^n$, respectively. The straight line is the linear fit for $n = 10$–15, while the dashed line gives the results for intermediate times $n = 4$–10.

an error bar of ± 0.010. For higher concentrations we made some estima-
tions for the asymptotic value of k and got values comparable to this one,
but with much larger error bars. We believe that the value of
$k = 0.183 \pm 0.010$ for time exponents $n = 10$–15 is realistic, because it is still
unclear if our data suffer from finite-size effects. This was the case in the
work of Pandey et al.[15] when these authors calculated the single-particle
critical exponent k as 0.175 because of a trend given by the last calculated
point.[27] That they were wrong was shown by Roman[17] on much larger
lattices.

A comparison of our data with the results of Heupel[19] shows that
Heupel simulated for too short times with too small accuracy. His total
particle concentration is about 1.25% of the whole lattice. His result for
the asymptotic exponent seems to be similar to our result for intermediate
times. Even for larger times on lattices of the same size, the finite-size effect
of Heupel's data could not be seen. Therefore we think that this
phenomenon was due to insufficient statistics, again resulting from too
small concentrations and lattices. Our result for the critical exponent does
not verify the Alexander–Orbach hypothesis.[3] Again, like the result of
Roman,[17] not only do static effects determine the diffusion behavior at p_c,
but also dynamic effects coming from the diffusion model. On the other
hand, within the available accuracy, the prohibition of double occupancy
does not change the exponent k, in agreement with earlier work.[19,22,23]

Plotting k versus $1/R$ for higher concentrations gives the result shown
in Fig. 2. A concentration-dependent behavior can easily be seen. In some
intermediate region the exponent becomes nearly constant with a value of
$k = 0.25 \pm 0.01$. The time range where this effect is visible depends on the
concentration. Looking at different lattice sizes and keeping the concentra-
tion constant, no size effect can be seen. This behavior of the exponent k
was not found by Heupel,[19] also probably due to his simulations at very
low concentrations.

We will now try to give a rough explanation of this phenomenon. For
a short time range after the beginning of the simulation a single particle
behaves as if it were alone on the lattice. Extrapolating the corresponding
data for an asymptotic behavior gives an asymptotic exponent of
$k = 0.20 \pm 0.01$. This behavior holds for all concentrations. Only the dura-
tion depends on the concentration. After the first crossover point we guess
that the systems behaves like a lattice gas at a concentration $\tilde{c}$, which
should somehow depend on c. In this intermediate time range, lattice gas
effects, i.e., correlations between the particles, are more important than the
effect of the disorder. On a regular lattice this would require an exponent
$k = 0.5$.[8,29] The reduction to a value around 0.25 could be due to the spe-
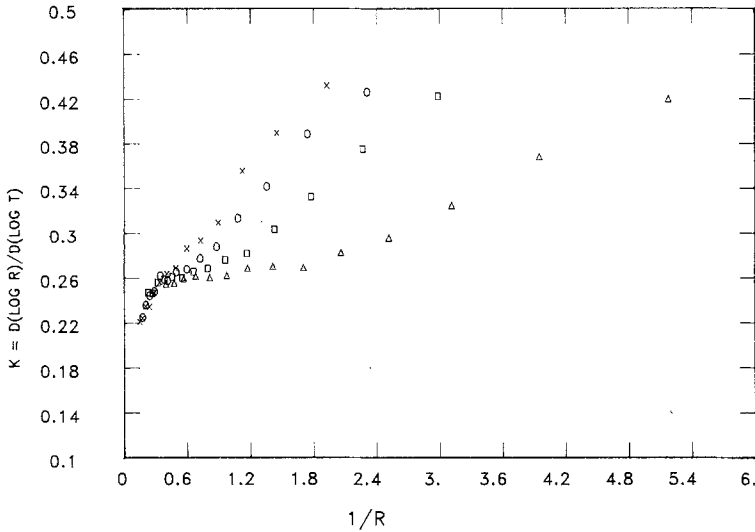cial properties of percolation lattices. The behavior of the correlation factor

Fig. 2.   The exponent k versus $1/R$ for lattice gases on three-dimensional percolation lattices at the percolation threshold at concentrations 0.3 ($\times$), 0.5 ($\bigcirc$), 0.7 ($\square$), 0.9 ($\triangle$).

for the tracer diffusion coefficient on lattices above the percolation threshold, as found by Braun and Kehr,[20] is possibly the clue for a more elaborate theory for the nearly constant exponent. After the second crossover point the behavior of the exponent becomes asymptotic again and tends to a universal value, independent of the concentration of the lattice gas.

In summary, we investigated the diffusion of lattice gases without double occupancy of sites on three-dimensional disordered lattices at the percolation threshold and found that the critical exponent is between the value of Pandey et al.[15] and the more accurate results of Roman[17] and hardly compatible with $k = 0.20$ from Alexander and Orbach.[3] Further, a new effect has been detected at intermediate times, which is a result of the interaction between the particles.

NOTE ADDED IN PROOF

The vectorizable algorithm[26] has been improved, so that an update rate of 0.33 μsec per update has been achieved. This is faster than the single particle algorithm[19] running on an CRAY X-MP/416. A reanalysis of the simulation data of Romans and our work, which takes the short time behavior of the particles into account, states that the critical exponent is $k = 0.200$ for several models. This result will be published by Sahimi and Arbab in this journal.

ACKNOWLEDGMENTS

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