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Classical diffusion, drift, and trapping in random percolating systems

R. B. Pandey*
Institute of Theoretical Physics, Cologne University, 5000 Koln 41, West Germany
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Monte Carlo studies for a biased diffusion are made on simple-cubic random lattices containing 180^3 and 256^3 sites with time steps up to 10^7. Above the percolation threshold, we observe diffusion for short times, and drift for long times, when the bias is below a characteristic value. For larger bias, a very slow relaxation, presumably to the asymptotic nonclassical behavior, is observed.

Recently, the problem of classical diffusion on random percolating clusters has been studied intensively.[1-7] In most of these current investigations one asks many questions: What is the power-law behavior of the root-mean-square (rms) displacement of a random walker? How does it approach its asymptotic value? How does it depend on the concentration p of the occupied sites? Earlier controversies[2] between the computer experiments and scaling theories on such questions seem to be settled now for unbiased diffusion on isotropic lattices.[7] It is well established that, in the power-law description for the rms displacement $R(t)$ with time t, in three dimensions,

$$R(t) \propto t^k \dots \quad (1)$$

The exponent $k=0$ for $p < p_c$ where $R(\infty)$ is the average radius of the clusters, $k=0.20 \pm 0.01$ at $p=p_c$, and $k=0.5$ for $p > p_c$, where Eq. (1) describes Einsteinian diffusion with adiffusivity D which goes to zero for $p \rightarrow p_c$, p_c being the percolation threshold. What happens when a biased field is switched on to cause the random walker to move with unequal probabilities $(1+B)/2$ and $(1-B)/2$ with $0 < B < 1$ in positive and negative directions, respectively? The random-walk motion diffuses the particle according to $R \propto \sqrt{t}$ while the biased field causes it to drift with $R \propto t$. When t is very small, diffusion dominates and when t is large, drift dominates. A crossover from diffusion to drift behavior thus occurs at about $t_{cr} \sim 1/(\text{bias field})$.[2] Barma and Dhar[8] have recently predicted that above the percolation threshold the drift velocity is nonmonotonic and vanishes above a critical value. On the other hand, Bottger and Bryksin[9] in a somewhat different model have shown that in high field, the current (presumably due to drift) decreases and goes to zero only in the infinite field (corresponds to $B=1$ here, and in Ref. 8). To examine the controversy on biased diffusion we perform a computer simulation to study various power laws, crossover, and relaxation due to competition of diffusion, drift, and trapping. Our simulations seem to support the suggestions of Bottger and Bryksin.[9]

The basic idea to model the problem of biased diffusion on computer is simple. As in our previous studies[7] of ordinary diffusion we first prepare the sample (called lattice realization) by distributing a fraction p of occupied sites randomly on a $L \times L \times L$ simple-cubic lattice (a quenched disordered lattice). A particle (random walker) is then placed on a randomly selected occupied site (called local origin). The biased probability B is set up to study the motion, for which a random number r is chosen randomly between 0 and 1 and is compared with B; if r is less than or equal to B then an attempt is made to move it to one of the randomly selected neighbors in the positive directions (i.e., in $+X$, $+Y$, or $+Z$ directions), otherwise, i.e., if $r > B$, the move is attempted to any of its six randomly selected neighbors. The bias B thus acts as a bias field pushing the walker into positive directions [with probability $(1+B)/2$] reducing its chance to turn back [in negative direction with probability $(1-B)/2$]. Note that this study is different from the other investigations of unbiased diffusion on the biased percolating clusters.[10] The random walker is moved to the neighboring site so chosen, if the site is occupied; otherwise it stays at the same position. Each attempt is counted as one time step. The process of selecting a neighboring site under the biased probability prescription and an attempt to move it is repeated again and again until the desired (preset) time step is reached. For reliable statistics at concentration p, the simulation is performed on several independent lattice realizations each with many independent local origins. The average mean-square displacement is calculated over these statistics and its value is recorded at various periods of intervals. For our studies here we perform the simulation mainly on samples 180^3 on a CDC Cyber-76 machine and on 256^3 samples using a CDC Cyber-205 vector machine. Apart from the biased field descriptions, the technical details may be found in Ref. 7.

The variation of rms displacement with time for various biased probabilities on $p=0.5$ random lattices is displayed in Fig. 1. The data for R in the "small time regime" (up to 10^5 time steps) were generated on 180^3 samples with 50 ar-

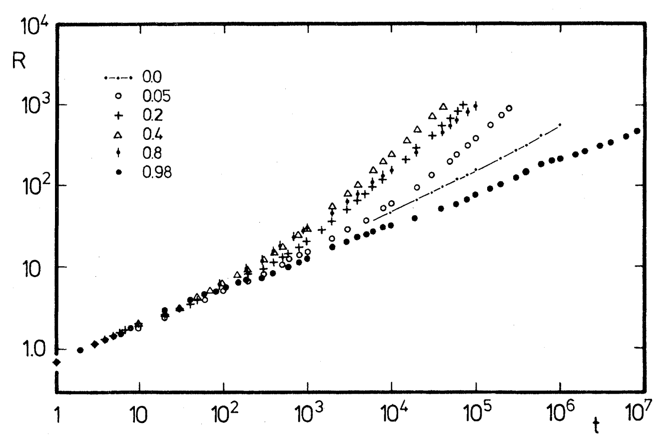

FIG. 1. Log-Log plots of the rms displacement R with time t at concentration $p=0.5$ for the bias $B=0.0$, 0.05, 0.2, 0.4, 0.8, and 0.98 with their respective symbols indicated in inset.

bitrary local origins each on 10 lattices using a CDC Cyber-76 machine; we use a CDC Cyber-205 machine for the data in "long time regime" (up to 10^7 time steps) on 256^3 samples with 512 local origins on two lattices. For most of our analysis here we have used the same statistics except for some better runs indicated in captions. The CDC Cyber-205 machine was about 11 times faster than ordinary CDC Cyber-76 machine. Several runs were made on smaller lattices (32^3 and 60^3) for $p > p_c$ but no appreciable finite size effects were observed to affect our conclusion based on our larger lattices. Note that R can often be much larger than the lattice size and that the periodic boundary conditions (used here) will not affect the mean-square displacements. At $B = 0.05$ for $p = 0.5$, as time grows, the diffusionlike ($\sqrt{t}$ variation of R) behavior is changed into driftlike (almost linear time dependence of R) behavior at about t_{cr} 5×10^4. The asymptotic behavior of R approaches sooner (i.e., the crossover time t_{cr} decreases) on further increasing the bias until a characteristic value above which the approach to asymptotic power-law behavior is slowed down. Finally, at the extreme bias $B = 1$, R approaches a constant value.

The picture becomes more transparent if we analyze an effective exponent $k_e[=d(\log R)/d(\log t)]$ as a function of time. We evaluate this exponent k_e in succesive interval of time, typically covering a decade. The resulting plots are shown in Fig. 2 for $p = 0.5$ far above $p_c = 0.3117$. On increasing the bias, the exponent k_e approaches its asymptotic value (1) faster until the characteristic bias (about $B = 0.4$) above which the approach to its asymptotic value is delayed on further increasing the bias. In high bias, B above 0.9, the variation of k_e with time becomes very slow. Although the data in the long time regime are fluctuating, the upward trend for k_e with t is rather clear. Note also that within the Monte Carlo time steps of our observation, the power-law variation of the rms displacements are neither diffusionlike nor driftlike, particularly in high bias.

A similar study at lower concentration $p = 0.3617$ $(= p_c \pm 0.05)$ gives the variation of the effective exponent k_e with time steps t as shown in Fig. 3. Compared with Fig. 2, one may say that the crossover and the power relaxation behavior remain qualitatively similar to those at $p = 0.5$. But now the characteristic bias seems to be reduced and the relaxation time for k_e to approach to its asymptotic value is increased. On further decreasing the concentration towards the critical value $p_c = 0.3117$, the relaxation becomes too slow to estimate a reliable trend of the asymptotic behavior within our computer time.

Thus, for the random-walk motion on the random simple-cubic lattice for $p > p_c$ in a biased field, our computer experiment indicates the existence of a characteristic biased field which depends on the concentration p. A bias below this characteristic value produces a crossover from diffusion to drift; the crossover regime depends on the bias. Above the characteristic bias we observe a decrease in R with increasing bias at constant time. This nonmonotonic behavior is in accord with the predictions of Barma and Dhar.[8] However, we have always found an increase of R with time t in our computer experiments consistent with the suggestions of Bottger and Bryksin[9] (to observe this trend we had to stretch our analysis to larger times up to 10^7 particularly for higher values of bias). Barma and Dhar,[8] on the other hand, predicted that the drift velocity vanishes for large enough values of the bias. This seems to be an artifact of their model where they consider the traps only due to branches (i.e., the long dangling ends of the clusters). Further, they model the infinite cluster by its backbone, which consists of long stretches of one-dimensional random

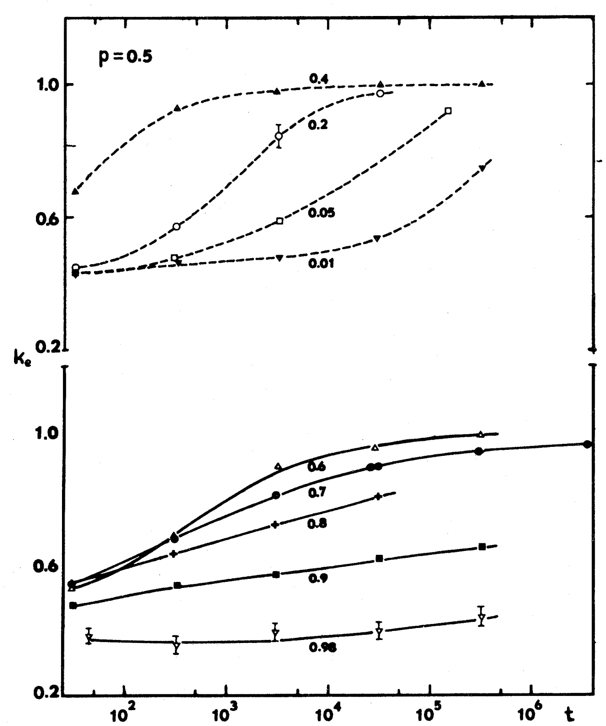

FIG. 2. Effective exponent k_e vs time step t at $p = 0.5$ on a semilogarithmic scale. Upper curves are for the bias below its characteristic value $B = 0.01$ (▼), 0.05 (□), 0.2 (○), 0.4 (▲); lower curves are for the bias above its characteristic value $B = 0.6$ (Δ), 0.7 (●), 0.8 (+), 0.9 (■), 0.98 (▽).

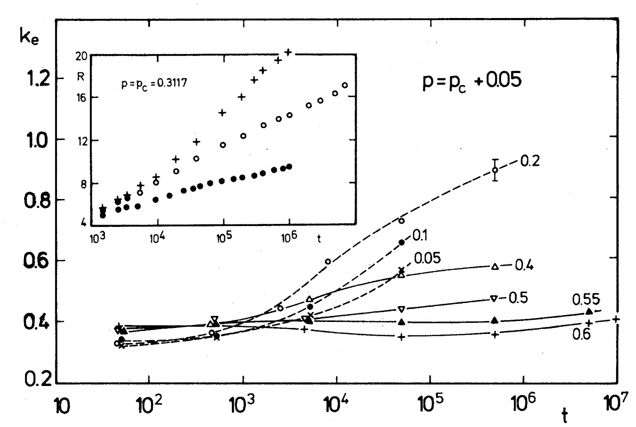

FIG. 3. Plots of k_e vs t at $p = 0.3617$ for $B = 0.05$ (×), 0.01 (●), 0.2 (○), 0.4 (Δ), 0.5 (▽), 0.55 (▲), and 0.6 (+). Inset figure shows the variation of R with t on semilogarithmic scale at $p_c = 0.3117$. At $B = 0.2$ (+) data up to 10^5 time steps were generated with the number of independent local origins $N = 80$ each on 20 lattice realizations, beyond $t = 10^5$, $N = 10$ with lattices on 180^3 sample. At $B = 0.5$ (○) for the data up to $t = 10^6$, $N = 50$ on 20 lattices of 180^3 samples beyond 10^6, $N = 512$ with 10 lattices on 256^3 samples. For $B = 0.8$ (●), $N = 50$ on 20 lattices on 180^3 samples.

paths between nodes.[8] This ideal situation, though necessary for the mathematical simplifications to obtain closed form analytic expressions, is certainly not correct for the concentration p much above p_c. Moreover, any power-law with $k_e < 1$ (which is in accord with our simulation) implies a vanishing velocity in the limit $t \rightarrow \infty$.

We know the bias field drives the random walkers forward in its positive directions. If the bias is large, the walkers reach quickly to the positive end of the cluster boundary or dangling ends of the clusters to which their local origins belong. The lower is the concentration p, the more ramified are the percolating clusters[11] and so are the chances for the random walker to hit the traps. In high bias, the random walkers have less probability to come out of the traps although they always attempt to turn back (in negative directions) with a finite probability $[(1-B)/2]$ for B less than one. Thus in high bias regime the disorder through its traps terminates the drift for a certain interval which we call the "trapping time" of the walker. This leads to a time varying power-law behavior with an effective exponent k_e approaching its asymptotic value only very slowly. The long time relaxation behavior seems to be some complex (perhaps logarithmic) functions in time, concentration, and bias. Possibly it is more complicated than the results of related studies on one-dimensional random system by Derrida and Pomeau.[12] Furthermore, while some theoretical arguments and computer simulations suggest[13] a nonclassical (neither diffusion nor drift) power-law behavior, even the longest run performed here shows metastability in high bias. One should, however, note that here the local metastability is due to competition between the bias and disorder (the ramified geometry of the clusters). Theoretical attempts (including the analogous multicritical studies[14]) are highly desired to combine all the competing effects, in particular at p_c. Further simulations are required specially for the study of biased diffusion on biased percolating clusters[15] to give more insight into the physics of this problem. We hope this report will stimulate further attention in this direction.

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*Present address: Cavendish Laboratory, Madingley Road, Cambridge, United Kingdom CB3 OHE.

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