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Diffusion of Interacting Particles on a Percolating Lattice

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The diffusion has been simulated by the "Monte Carlo method" on a random lattice. As in the "ant in the labyrinth" problem the particles move by stepping to allowed, randomly chosen neighboring fields. The particle interaction has been defined by the constraint that only one particle can occupy a site at a time. Biased diffusion means that one of the directions will be chosen with a greater probability than the others. It was shown that, with an increasing number of "walkers," the displacement of the particles first of all increases to a maximum value and then decreases. This "filling-up" effect will not occur with small bias fields and on lattices with a high concentration of allowed sites.

KEY WORDS: Percolation; Monte Carlo simulation; ant in the labyrinth; diffusion; interaction; trapping; "filling up."

1. INTRODUCTION

By describing the diffusion as a random movement the Monte Carlo method can be used for simulation. We can find a lot of such studies in the physical literature of the last years.[1-3] Lattices are used—in this study a simple cubic one—where the sites are only allowed to be occupied with the probability p, the allowed sites are chosen randomly. A particle can move one step to a neighboring field, if it is allowed to do so (ant in the labyrinth[1]). For a lattice where the probability of allowed sites p is such that $p > p_c$ and all directions can be chosen with an equal probability the displacement–time relationship is given by[4]

$$R = \langle \Delta R^2 \rangle \propto t^{0,5}$$

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In general this relationship is described as[5]

$$R \propto t^k$$

At the percolation threshold p_c the exponent is equal to 0.2.[6] For $p < p_c$ only finite clusters exist.[5,7] If the diffusion is biased by a weak "wind", i.e., one of the directions will be chosen with a slightly greater probability than the others, then there will eventually be a linear relationship between displacement and time: the particle will drift with a constant velocity, the exponent k is equal to 1.0.[8,9] The drift leads first of all to a greater particle displacement as the bias field grows. However, beyond a certain field strength, the displacement decreases as the bias field becomes stronger.[8-11] The reason of this is that dangling ends in the direction of the wind become effective traps.[8]

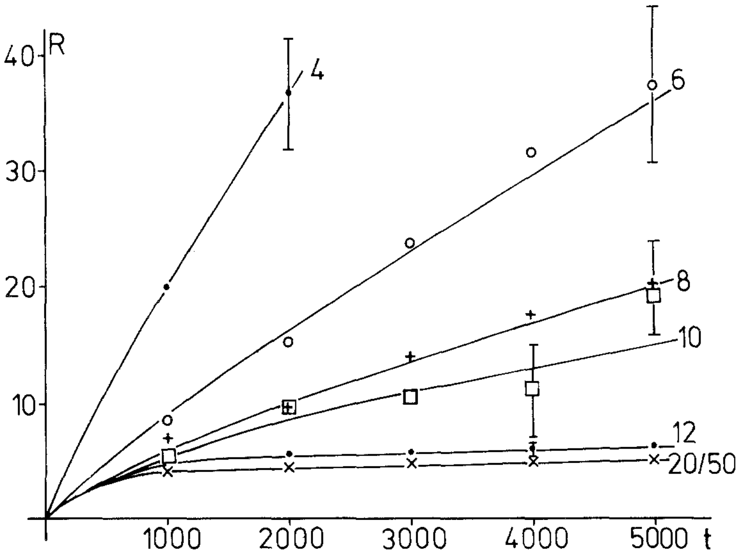
In this study the particles were not independent of each other in that two or more particles could not occupy a single site simultaneously. Under this condition of interaction the value of the exponent k in the R–t relationship, for unbiased diffusion at the percolation threshold, could be found. The motion of each particle was followed as a function of time.

The central aim of this study was to analyze the relationship between the displacement of the particles and the number of particles on a lattice. It has been shown that, using a medium bias field (BF = 0.5) and a medium probability for allowed sites ($p = 0.5$), the mean displacement of particles does not immediately decrease as more particles are introduced to the lattice. Instead, contrary to what might be expected from the hindrance due to particle interaction, the displacement first increases to a maximum value when the number of particles is 10%–20% of the number of the free sites.[12]

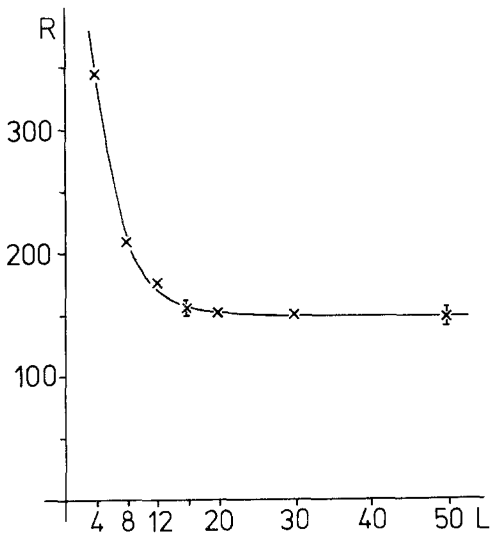
This research deals with the relationship between this "filling-up" effect of the first growing of the displacement and the combination of bias field/probability of allowed sites.[13]

2. PROCEDURE

The simulations were made on a CDC-CYBER 76 machine using a program similar to that used in the study of Pandey *et al.*[6] However, unlike in Pandey's study,[8] the bias field was defined differently: BF is the probability that a step would be made in a specific direction (1-BF) the probability that the step would be made in one of the six equally likely directions.



(a)



(b)

Fig. 1. Displacement R using different dimensions of the lattice: (a) $p < p_c$, R versus time t (the numbers indicate the linear size of the lattice, $p = 0.3$, BF $= 0.4$, $N = 1$); (b) $p > p_c$, R versus linear size of the lattice L ($t = 5000$, $p = 0.7$, BF $= 0.4$).

2.1. Values and Error Estimations

Since the random result from one simulation would not have been useful, the mean value from a series of independent investigations was used. Several lattices were build up and in each the displacement of the "blind ants"[5] was calculated. For each sequence an average displacement and scattering value were then calculated from the results of the different lattices. Using these results, the exponent k and the velocity v of each sequence were found. Our effective exponent $k(t)$ is defined as: $d(\log R)/d(\log t)$ the velocity $v(t)$ as: dR/dt.

2.2. Size of the Lattice

The program used is based on a finite lattice, that has been made infinite by periodical boundary conditions. The effects due to the fact that the basic lattice had finite dimensions were investigated; the results are shown in Fig. 1.

Since linear dimensions greater than $L = 20$ produced no appreciable change, this value was most frequently used. A greater value of L would have required a greater number of particles and a greater calculation time.

3. RESULTS

3.1. Exponent k at the Percolation Threshold

Figure 2 shows this exponent as a function of the reciprocal value of the displacement. With increasing displacement the exponent decreases and can be extrapolated to

$$k \approx 0.199$$

when R is going to infinity.

This value is identical to that calculated in the study without particle interaction.[6] A greater number of particles ($N = 249$, that is nearly 10% of the free sites) leads to comparable results. A similar effect was found by Amitrano *et al.*[14]

Without particle interaction the deviation at small values of $1/R$ was also present and it was argued, that this deviation depends on the size of the basic lattice. In a smaller lattice of $L = 10$ the deviation occurs with a smaller displacement and justifies this assumption.

3.2. "Filling-up" Effect

Figure 3 shows the displacement normalized by the value of one particle, using a fixed probability of allowed site $p = 0.5$ and different bias

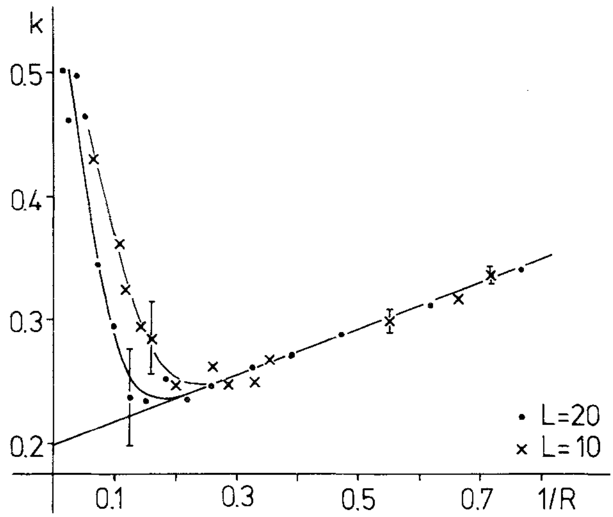


Fig. 2. Exponent k at the percolation threshold with interacting particles. Exponent k versus $1/R$ ($p = p_c$, BF = 0): · represents the results on a lattice with the linear dimension $L = 20$ and number of particles $N = 100$; × shows the results using $L = 10$ and $N = 13$.

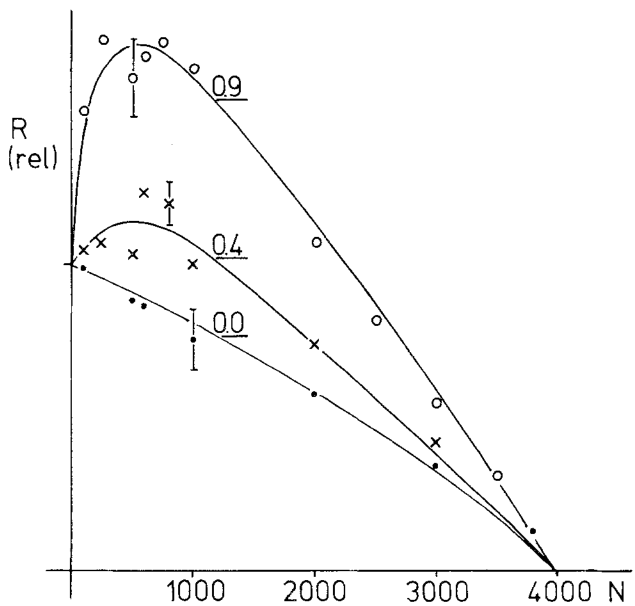


Fig. 3. Filling-up effect using fixed probability $p = 0.5$ and variable bias fields BF. R (normalized by the value gained with $N = 1$) versus number of particles N ($L = 20$, $t = 5000$, the numbers indicate the values of BF).

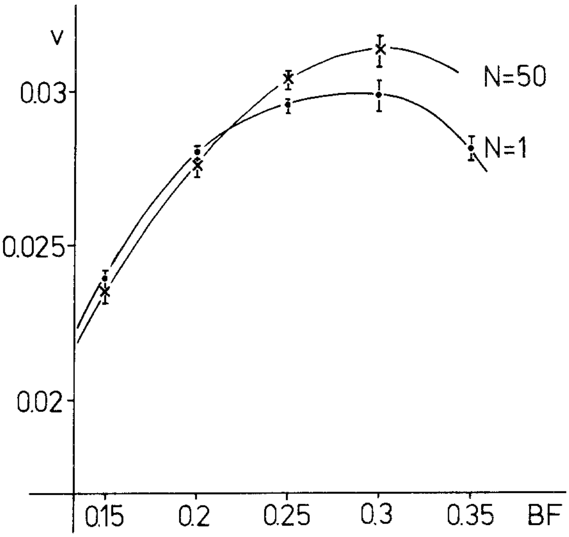


Fig. 4. The end of the filling-up effect near BF = 0.22. Final velocity v versus bias field BF [$L = 20$, $p = 0.5$, $t = 30000$, $N = 1$ (·), $N = 50$ (×)].

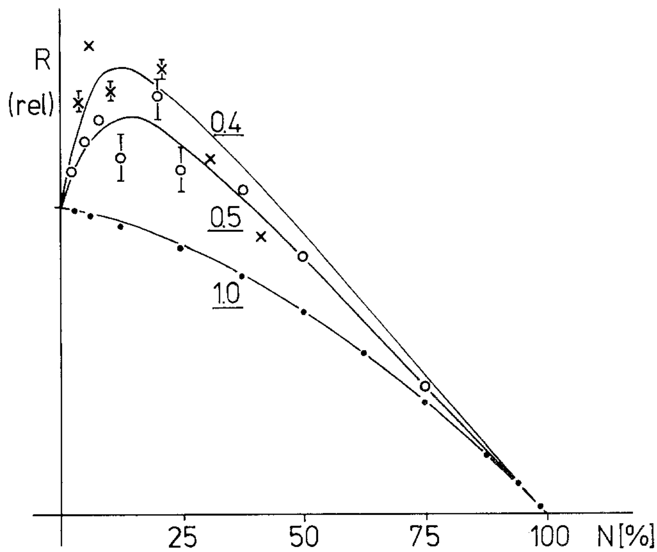


Fig. 5. Filling-up effect using fixed bias field of BF = 0.5 and variable probabilities of allowed sites. R (normalized by the R of one particle) versus the fraction of free sites occupied by particles ($L = 20$, $t = 5000$, the numbers indicate the value of p).

fields with a bias factor BF, as the function of the number of particles. The increase in relative R values will be stronger with greater bias fields.

Figure 4 shows the dependence of the final velocity v (when k is equal to 1) on the bias field using 1 and 50 particles. The final velocity is a useful value, because it shows the constant increase of the displacement with the time. As shown in Fig. 4 there is no "filling-up" effect with a bias factor weaker than $\mathrm{BF} = 0.22$ (using $p = 0.5$).

Using a bias field of the fixed value of $\mathrm{BF} = 0.5$, the filling-up effect will be stronger with a smaller probability of allowed sites (see Fig. 5); Fig. 6 demonstrates that this effect occurs only using a probability less than $p = 0.66$.

The results of the investigations into the effect of different combinations of the two parameters are shown in Fig. 7. As there only was a short time for the investigations it was impossible to give certain answers for all cases, but the tendency is evident: greater values of the probability of allowes sites require a stronger bias field in order to find the "filling-up" effect. The border is nearly a straight line in the BF versus p plot.

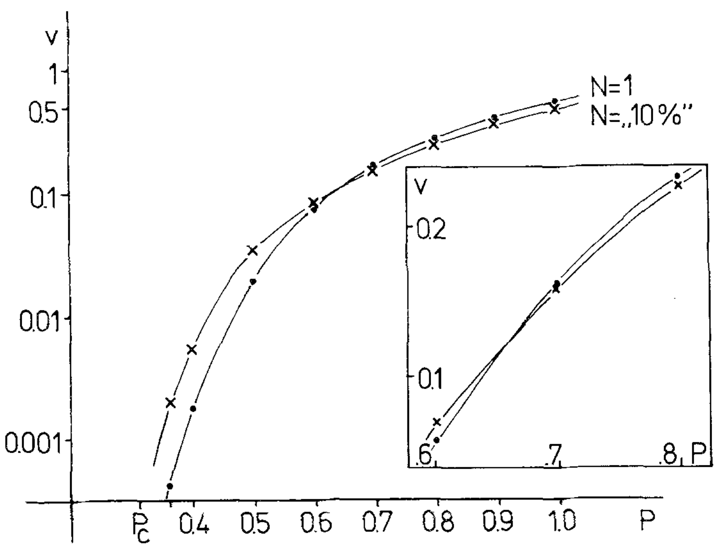


Fig. 6. The end of the filling-up effect near $p = 0.66$. Final velocity v versus probability p [$\mathrm{BF} = 0.5$, $L = 20$, $t = 20000$, $N = 1$ ($\cdot$), N is 10% of free sites ($\times$), the size of the symbols shows the scattering].

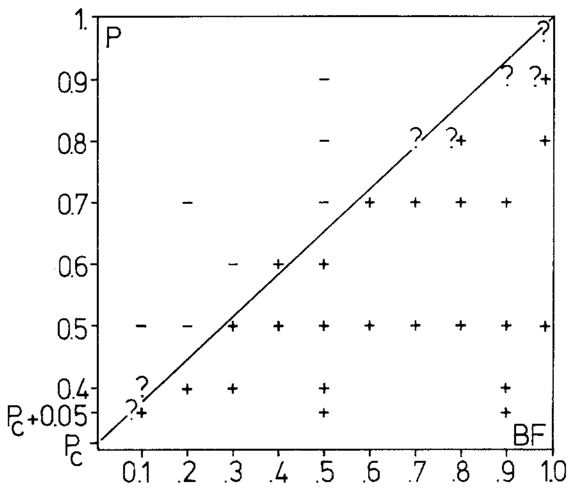


Fig. 7. All combinations of the parameter BF and p are represented by a point in this diagram. + indicates the filling-up effect, − indicates the absence of this effect, ? indicates no exact answer can be given. The straight line demonstrates the nearly linear character of the border of the filling-up effect.

4. INTERPRETATIONS

With a greater number of particles put into the lattice, some of them will stay in the traps and will therefore reduce the effects of the traps on the others, i.e., the traps are filled up. This leads to a greater mean displacement of each individual particle than reached by only one of them.[12] With smaller bias factors we see the prevalence of the drift (see Fig. 4) and small effects of trapping; the filling-up is unimportant.

Traps arise in the combination of dangling ends with a prevailing direction. With a small number of allowed sites we have a complicated structure and even small bias fields produce traps. Using a great number of allowed sites we need stronger bias fields in order to gain effective traps.

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REFERENCES

1. P. G. de Gennes, *La Recherche* 7:919 (1976).
2. D. Stauffer, *Introduction to Percolation Theory* (Taylor and Francis, London, 1985).

3. Y. Gefen, A. Aharony, and S. Alexander, *Phys. Rev. Lett.* **50**:77 (1983).
4. D. Ben-Avraham and S. Havlin, *J. Phys. A* **15**:L691 (1982).
5. C. Mitescu and J. Roussenq, *Ann. Isr. Phys. Soc.* **5**:81 (1983).
6. R. B. Pandey, D. Stauffer, A. Margolina, and J. G. Zabolitzky, *J. Stat. Phys.* **34**:427 (1984).
7. F. Family and P. J. Reynolds, *Z. Phys. B-Cond. Matt.* **45**:123 (1981).
8. R. B. Pandey, *Phys. Rev. B* **30**:489 (1984).
9. E. Seifert and M. Süssenbach, *J. Phys. A* **17**:L701 (1984).
10. M. Barma and D. Dhar, *J. Phys. C* **16**:1451 (1983).
11. H. Böttger and V. V. Bryksin, *Phys. Stat. Sol. B* **113**:9 (1982).
12. M. Przyborowsky and M. v. Woerkom, *Eur. J. Phys.* (in press).
13. The presented study is the short version of L. Heupel, Staatsexamensarbeit 1985, Univ. of Cologne.
14. C. Amitrano, A. Bunde, and H. E. Stanley, *J. Phys. A* **18**, Letters (1985).

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