MOLECULAR PHYSICS REPORTS 9 (1995) 86-91

THE DRIFT VELOCITY IN PERCOLATING SYSTEMS

CZESŁAW OLEKSY

Institute of Theoretical Physics, University of Wrocław,
Pl. Maksa Borna 9, 50-204 Wrocław, Poland

ABSTRACT: We calculate the drift velocity for a random walk on percolation clusters in the presence of an external field from the steady-state solution for site probabilities. We find that the drift velocity decreases rapidly after reaching a maximum. Close to the percolation threshold the decrease is exponential and we observe at strong field that the velocity can be reduced by over million times.

1. INTRODUCTION

Diffusion in disordered systems under the influence of a biased field exhibits complex behaviour [1-7]. An interesting problem is the existence of drift in biased diffusion on percolation clusters. White and Barma [8] calculated the drift velocity on one-dimensional lattice with random-length branches and on the diluted Bethe lattice. In both cases they found that the drift velocity vanishes once the external field exceeds a critical value. Barma and Dhar [9] assuming an exponential distribution for the particle density in the steady state on percolation clusters showed that the drift velocity vanishes above the percolation threshold for large enough values of the field. Pandey [10] performed a MC simulation of a random walk on a 3-D random lattice in a biased field. His simulations support the suggestions of Botteger and Bryskin [11] that the drift velocity goes to zero only for an infinite biased field.

In this paper we study the dependence of the drift velocity on the biased field by finding the numerical solution of the steady-state on finite percolation clusters above the percolation threshold.

2. BIASED DIFFUSION ON PERCOLATION CLUSTERS

In a previous paper [12] we described the diffusion on percolation clusters using a random Lorentz model (RLM) [13]. Lattice sites in the RLM are occupied by particles with probability p and impurities with probability $1-p$. The walker performs a pure random walk over cluster sites and can also visit sites occupied by impurities which play role of reflectors, i.e. when the walker reaches an impurity site then it is reflected backward to the cluster site visited previously. Hence the motion of the walker is limited to sites of single cluster and sites occupied by impurities which are nearest neighbours of the cluster. It is worth noting that in the most popular model,

"the myopic ant in a labyrinth" [1], the walker cannot jump to sites with impurities and the transition rates change from site to site.

In this paper we modify the RLM for the biased percolation problem on a square lattice. We do that by changing a pure random walk into a biased random walk over percolation cluster sites. In other words the transition rates are the same for each cluster site but they depend on the biased field. The bias is chosen to be constant at cluster sites and it pushes the walker in a positive direction with probability $p_+ = (1+B)/4$ but reduces the chance for go in a negative direction with probability $p_- = (1-B)/4$. The zero bias corresponds to $B = 0$ whereas $B = 1$ denotes infinitely large bias. There is no influence of bias on sites occupied by reflectors.

The method we use to calculate the drift velocity of the walker is based upon a steady-state solution for site probabilities, $P(\mathbf{r}, i, N)$, finding the walker after N steps at site $\mathbf{r}$ with velocity directed along lattice vector $\mathbf{e}_i$. Assuming the lattice constant and the time step equal to unity we find that the instant velocity of the walker is one of the four vectors: $\mathbf{e}_{\pm 1} = (\pm 1, 0)$, $\mathbf{e}_{\pm 2} = (0, \pm 1)$. The site probabilities for the steady state fulfils the following equation

$$P_s(\mathbf{r}, i) = \sum_j T_{ij}(\mathbf{r}) P_s(\mathbf{r} - \mathbf{e}_j, j) \tag{1}$$

where an element of the transition matrix, $T_{ij}(\mathbf{r})$, denotes the probability of changing the velocity from $\mathbf{e}_j$ to $\mathbf{e}_i$ after a jump to site $\mathbf{r}$. At cluster sites $T_{1j} = T_{2j} = p_+$ and $T_{-1j} = T_{-2j} = p_-$; whereas, at a site occupied by a reflector the walker changes the sign of the velocity with probability equal to 1: $T_{ij} = \delta(\mathbf{e}_j + \mathbf{e}_i)$.

The equation (1) can be solved iteratively for a given cluster. We start from a steady-state for zero bias which is easy to find exactly [12]. Putting a small bias we solve Eq. (1). Then the bias is increased and a new steady-state is calculated using the previous solution as the initial state. Hence steady-states are generated from the initial state (at $N = 0$) in which all starting positions and directions for the walker have the same probability. We apply the overrelaxation method to solve Eq. (1) (note that for zero bias it resembles the discrete Laplace equation). We stop the iterations when relative difference of site probabilities at two successive iteration is smaller than $\varepsilon = 10^{-4}$ or when the number of iteration exceeds 10^5. In the latter case we do not accept the solution of Eq. (1) as a steady-state one.

The percolation clusters we used to calculate steady-states were generated on the square lattice of 119^2 sites by the MC method, i.e. lattice sites are occupied by particles with probability p and by impurities with probability $1-p$. We used periodic boundary conditions similar to those in the MC simulations of Pandey [10].

After finding the steady-state for a given value of biased field we calculate the drift velocity

$$\mathbf{v}_d = \sum_{\mathbf{r},j} P_s(\mathbf{r},j)\mathbf{e}_j \tag{2}$$

and average over 10 clusters. Calculations were performed above the percolation threshold ($p_c = 0.593$) for the following values of probabilities: $p = 0.60, 0.65, 0.70, 0.8$.

3. DISCUSSION

The drift velocity is a not monotonic function of the bias (see Fig. 1). It changes linearly at small bias, reaches a maximum, and decreases very fast for a strong bias.

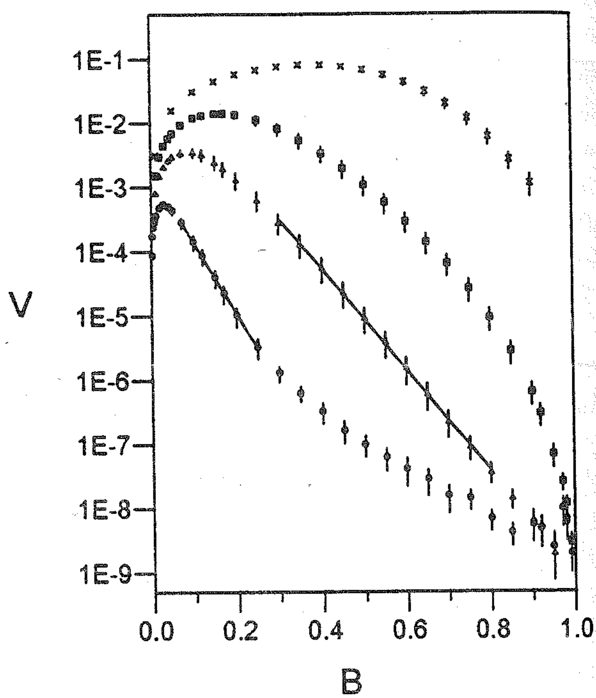

Fig. 1. Log-log plots of the drift velocity vs bias above the percolation threshold. Circle, triangle, square and cross represent data for probability $p = 0.60, 0.65, 0.70$ and 0.80, respectively.

Close to the percolation threshold, $p = 0.65$, the drift velocity decreases exponentially and for $B = 0.9$ its value is reduced by over a million times. We observe the noise in the behaviour of the velocity for a very strong bias due to the accuracy (ε) of the steady-state solution. We discuss this problem below. The maximum of the drift velocity decreases very fast as the probability p approaches the critical value p_c. For example, $v_{max} = 8.1 \times 10^{-1}, 1.4 \times 10^{-2}, 3.5 \times 10^{-3}$ and 5.4×10^{-4} for $p = 0.8, 0.7, 0.65$ and 0.60, respectively. The position of the maximum moves toward zero bias as p goes to p_c from above. In the region of small fields, the drift velocity is a linear function of the biased field, $v_d \approx v_L B$. The linear coefficient v_L decays as p approaches the critical value p_c (see Fig. 2).

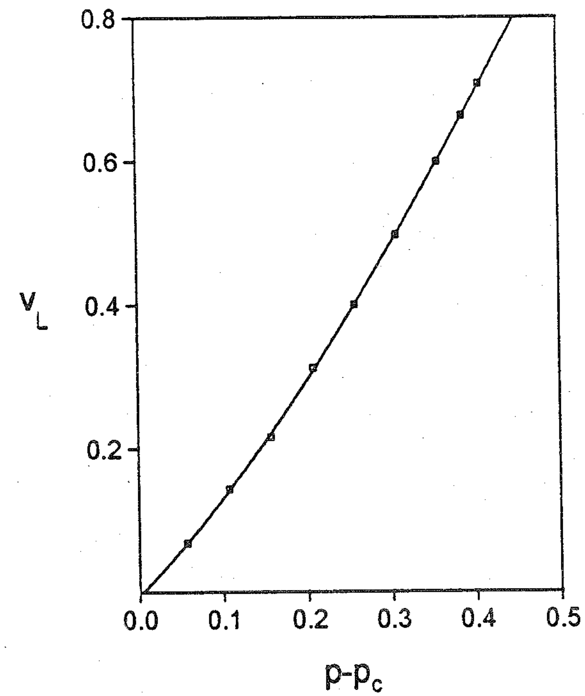

Fig. 2. The linear coefficient of the drift velocity vs $p - p_c$. The symbols denote the results of simulations and the line is a parabolic fit.

A main reason for the vanishing of the drift is the trapping of the walker in the dangling-ends or backbends of the cluster. In order to discuss this problem we calculated the density of probability,

$$P_s(\mathbf{r}) = \sum_j P_s(\mathbf{r},j)\,,$$

of finding the walker at site $\mathbf{r}$ in the steady-state. The interval (0, 1) has been covered by a sequence of intervals $\{l_1, l_2, \ldots\}$ and we counted the fraction of site probabilities $P_s(\mathbf{r})$, in the interval

$$l_n = \left(\left(\frac{2}{3}\right)^n, \left(\frac{2}{3}\right)^{n-1}\right).$$

The results for $p = 0.65$ are plotted in Fig. 3. Density of site probabilities (DOSP) has a sharp maximum for small bias ($B = 0.05$). Note that at zero bias all sites have equal probability. As the bias increases the maximum of the DOSP decreases and its position moves towards very small probabilities. This means that a majority of sites has a very small probability $P_s(\mathbf{r})$. On the other hand, the DOSP is stretched out towards higher probabilities as the bias increases; this means that there is a very small fraction of sites with a significant value of $P_s(\mathbf{r})$. These sites play the role of traps. The walker can be trapped in a dangling end with a probability which depends on its size and the value of biased field. A trapping centre, in our model, consists of a single cluster site and two or three reflectors in its nearest neighbourhood blocking motion along the field direction. Hence the walker in the trapping centre does not rest but oscillates between the site and reflectors, and its mean velocity is equal to zero. We observed that, in a single cluster, there are several dominating trapping centres (each centre has a probability of order 10^{-1}) and the probability of finding the walker in these centre is between 0.7 and 0.9 for clusters with $p = 0.65$ and $B = 0.95$.

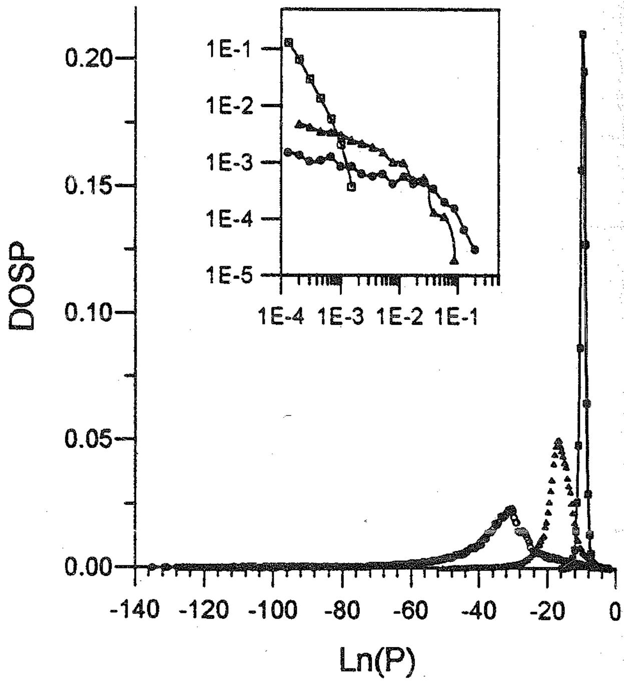

Fig. 3. The density of site probabilities in steady-states above the percolation threshold $p = 0.65$. The square, triangle and circle represent data for the biased field 0.05, 0.40 and 0.95, respectively. In the inset, the DOSP in region of high probability is shown on a log-log plot.

Probabilities which contribute to the drift velocity may change from 10^{-1} to 10^{-50} for a strong biased field (see Fig. 3). The error in the calculation of the site probability depends on ε: $\delta P(\mathbf{r}, j) \sim \varepsilon P(\mathbf{r}, j)$. Hence the accuracy of the drift velocity in our method depends on ε and the magnitude of the higher site probabilities. We estimate the accuracy in the case of a strong bias and close to the percolation threshold from 10^{-8} to 10^{-6}. The convergence in our method is slow for values of bias which result in a rapid decay of the drift velocity. For example the number of iterations needed to get the steady-state solution with $\varepsilon = 10^{-4}$ was more than 10^4 for clusters very close to the percolation threshold.

Finally we comment on the problem of diffusion-like behaviour (for small times) and drift-like behaviour (for long times) in biased diffusion. The contribution to the mean square displacement $R(N)$ of a walker coming from drift is $v \times N$. Thus the number of steps in a MC simulation should be of the order of 10^7-10^9 to observe drift-like behaviour in a strong biased field.

(Received 6 February 1995)

References

[1] S. Havlin, D. Ben-Avraham, Adv. Phys. **36**, 695 (1987).
[2] S. Havlin, A. Bunde, Y. Glaser, H. E. Stanley, Phys. Rev. A **34**, 3492 (1986).
[3] S. Havlin, A. Bunde, H. E. Stanley, D. Movshovitz, J. Phys. A **19**, 1693 (1986).
[4] Y. Gefen and I. Goldhirsh, J. Phys. A **18**, L1037 (1985).
[5] D. Stauffer, J. Phys. A **18**, 1827 (1985).
[6] Gi Ok Kim, Jong Hoon Oh, Jong-Jean Kim, J. Phys. A **20**, 1905 (1987).
[7] M. R. Dudek, W. M. Trochimczuk, R. Wycisk, J. Membram Sci. **67**, 273 (1992).
[8] S. R. White and M. Barma, J. Phys. A **17**, 2995 (1984).
[9] M. Barma, D. Dhar, J. Phys. C **16**, 1451 (1983).
[10] R. B. Pandey, Phys. Rev. B **30**, 489 (1984).
[11] H. Bottger and V. V. Bryskin, Phys. Stat. Sol. (b) **113**, 9 (1982).
[12] Cz. Oleksy, Physica A **205**, 487 (1994).
[13] J. Kortus and Cz. Oleksy, J. Phys. A **25** 1093 (1992).