DIFFUSION IN A 2D BOND PERCOLATION MODEL. A MONTE CARLO SIMULATION

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A Monte Carlo computer simulation of a simple stochastic hopping model is presented. The velocity autocorrelation function and the diffusion coefficient are analyzed and compared with the results obtained by using kinetic theory. The theory and the simulation agree within the statistical error.

1. Introduction

The long time behavior of equilibrium correlation functions has been one of the most exciting and studied problems in statistical mechanics for the last years [1]. From a theoretical point of view, it has been analyzed using different approaches, such as mode-coupling theories and kinetic theory. Perhaps, the most interesting result is the understanding of a strong long time tail observed by Alder and Wainwright [2] in molecular dynamics simulations. Nevertheless, a definitive check of the agreement between the theoretical predictions and the computer simulation results is still lacking [3].

In the last few years, Ernst has carried out an extensive study of several simple stochastic hopping models [4], using methods of kinetic theory. In the present paper we report some computer simulation results for one of those models, namely the so-called two-dimension bond percolation model. In short, it can be described as independent random walkers moving in a random square lattice with a concentration c of missing bonds. The quantity we will focus on is the velocity autocorrelation function (VACF), defined as

$$\Phi(t) = \langle V_x(0) V_x(t) \rangle , \tag{1}$$

where the average is taken over both trajectories and lattice realizations. The time dependent diffusion coefficient is given by

$$D(t) = \int_0^t \mathrm{d}s\, \Phi(s) , \tag{2}$$

while the static diffusion coefficient is $D(\infty)$.

The main theoretical results are the following ones. The short time behavior of the VACF reads [5]

$$\Phi(t) = \tfrac{1}{4}(1-c)\delta_+(t) - \tfrac{1}{8}c(1-c) + \tfrac{1}{32}c(1-c)(3-c)t + \mathrm{O}(t^2) , \tag{3}$$

where $\delta_+(t)$ is a Dirac delta-function on positive time. Here and in the following, we take the edge of the unit cell as the length unit, and the inverse of the jump frequency as the time unit. On the other hand, for finite and long times the behavior is given as a series expansion

$$\Phi(t) = \Phi^{(0)}(t)c + \Phi^{(1)}(t)c^2 + O(c^3) . \tag{4}$$

Van Velzen and Ernst [6] have obtained the Laplace transforms of $\Phi^{(0)}(t)$ and $\Phi^{(1)}(t)$ and have evaluated them by numerical inversion for a wide range of times. In addition, the long time behavior is given by [7]

$$\Phi^{(0)}(t) = -(1/2\pi t^2)\{1 + (4/\pi)\ln(t/\tau_0)/t + \mathrm{O}((\ln t)^2/t^2)\} , \tag{5}$$

and

$$\Phi^{(1)}(t) = -(\beta_1/2\pi t^2)[1 + \mathrm{O}((\ln t)/t)] . \tag{6}$$

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In these expressions, $\tau_0=0.1434$, and $\beta_1=3.7713$. The static diffusion coefficient has been found to be [7]

$$D(\infty)=\tfrac{1}{4}[1-2c+\alpha_2 c^2+O(c^3)]\,, \tag{7}$$

with $\alpha_2=-0.21075$.

Eqs. (5) and (6) show a long tail of the VACF decaying as t^{-2}, that is characteristic of (2D) Lorentz models.

2. Computer simulation

We have carried out Monte Carlo (MC) simulations of the above model. A similar study for a site model has been performed by Frenkel [8]. A bond model has already been simulated by Haus et al. [10]. Nevertheless, as they themselves claim, their results for the VACF had a preliminary character due to the low statistics. In our simulations the random walkers make a step each unit of time, while in the theoretical considerations the time is taken as a continuous variable. Nevertheless, one can establish an exact relationship between continuous and discrete quantities [9]. Namely, one has

$$\Phi(t)=\tfrac{1}{2}\Phi_0\delta_+(t)+e^{-t}\sum_{n=0}^{\infty}\frac{t^n}{n!}\Phi_{n+1}\,, \tag{8}$$

$$D(t)=e^{-t}\sum_{n=0}^{\infty}\frac{t^n}{n!}D_{n+1/2}\,, \tag{9}$$

where Φ_n and $D_{n+1/2}$ are the discrete VACF and diffusion coefficient, respectively, at the nth timestop. They can be expressed in terms of the discrete square mean displacement through the relations

$$\Phi_n=D_{n+1/2}-D_{n-1/2}$$
$$=m_{n+1}-2m_n+m_{n-1},\quad n\geqslant 1\,, \tag{10}$$

$$\Phi_0=2D_{1/2}=2m_1\,, \tag{11}$$

$$m_n=\tfrac{1}{2}\langle(x_n-x_0)^2\rangle\,. \tag{12}$$

We notice that comparison of eq. (3) with eq. (8) gives the following exact expressions for the first few discrete VACFs: $\Phi_0=\frac{1}{2}(1-c)$, $\Phi_1=-\frac{1}{8}c(1-c)$, $\Phi_2=-\frac{1}{32}c(1-c^2)$.

In our simulations we have considered a concentration $c=0.05$. To compute the averages, the invariance under time translation of the VACF has been exploited. We have generated about 500 square lattices of size 500×500 with randomly distributed missing bonds. In each realization the path of a test particle has been followed during a number of 2×10^6 timesteps typically. More precisely, each value of the discrete VACF up to $n=100$ has been averaged over 9.91×10^8 single values. The side of the lattice is about one half the (theoretical) mean square displacement of the particle after 2×10^6 timesteps. We have checked that in this case there are no relevant effects due to the finite size of the system.

Once the Φ_n, $n\leqslant100$, are known, we make use of eq. (8) to evaluate $\Phi(t)$. Of course, this implies a truncation error, so that reliable values of $\Phi(t)$ can be expected only up to a certain finite value of time.

3. Results

As a test of our MC data, we have compared in table 1 the exact and the observed values of the first few Φ_n. It is seen that the computer results are in good agreement with the theory, within the statistical error. Here and in the following the statistical error is estimated by taking 10 independent samples of a typical size $N=10^8$ trajectories, and computing from them the mean square error corresponding to this sample size. By assuming that the error is proportional to $N^{-1/2}$ we have estimated the error associated to $N=9.91\times10^8$. From a practical point of view, we have found this source of error to be more important than the one associated to the truncation in eq. (8).

The time behavior of the VACF for $0<t\leqslant1$ is shown in fig. 1. Also, we have plotted $\Phi^{(0)}(t)$ and $\Phi^{(0)}(t)+c\Phi^{(1)}(t)$ as obtained from kinetic theory. It is seen that $\Phi^{(0)}$ is not quantitatively sufficient for a concentration $c=0.05$. On the other hand, the MC results are indistinguishable from the theoretical

Table 1
First few values of the discrete VACF obtained in the MC simulation. The available values from kinetic theory are also included.

n	Exact	MC
0	0.475000	0.47500 ± 0.00002
1	-5.9375×10^{-3}	$-(5.92\pm0.02)\times10^{-3}$
2	-1.5586×10^{-3}	$-(1.56\pm0.02)\times10^{-3}$
3		$-(1.50\pm0.01)\times10^{-3}$
4		$-(5.8\pm0.1)\times10^{-4}$
5		$-(6.8\pm0.1)\times10^{-4}$

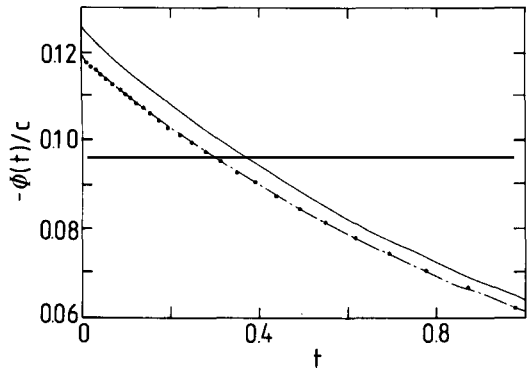

Fig. 1. Time dependence of the VACF for $c=0.05$, divided by the concentration of missing bonds, for times $0<t\leqslant 1$. The solid (broken) curve represents the kinetic theory result up to the first (second) order in c. The Monte Carlo data are represented by circles (which are larger than the error bars).

curve including quadratic terms.

To analyze the long time behavior of the VACF, we plot $\Phi(t)$ versus t^{-2} in fig. 2, as suggested by eqs. (5) and (6). As before, the linear and quadratic kinetic theory predictions are also shown. Again, the MC data clearly deviate from the first order approximation to $\Phi(t)$. The difference with respect to the second order approximation is comparable to or smaller than the error bars, so that one cannot conclude whether it is due to higher order effects. It is worth to notice that, although fig. 2 apparently shows an almost linear behavior, the pure t^{-2} decay (represented up to the second order by the straight line) is reached on the scale of the figure only for $t\geqslant 70$. Consequently, it would not be legitimate to use the MC data shown in fig. 2 to get the coefficient of t^{-2} [8]. In order to see whether a logarithmic term correction similar to that of eq. (5) can be identified from the MC data, we have plotted $2\pi t^2\Phi(t)$ versus $t^{-1}\ln(t/\tau_0)$ in fig. 3. It is observed that the curves exhibit a maximum at $t\approx 10$. This time can be chosen as a natural criterion to define short and long time behavior at a qualitative level. The location of the maximum shifts to longer times as the concentration increases. Fig. 3 also shows that although the MC data are compatible with a logarithmic contribution to the long-time tail of the VACF, they are not accurate enough to allow its identification.

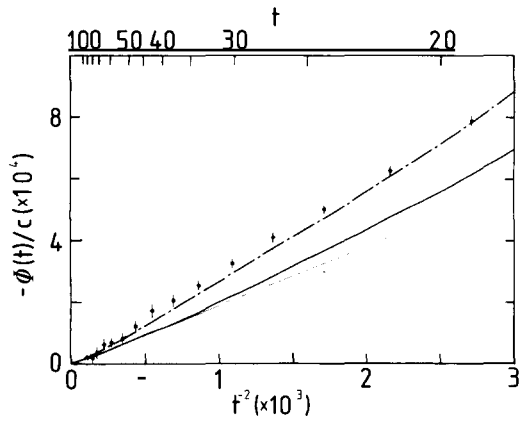

Fig. 2. Plot of the VACF versus t^{-2}. The curves and the circles have the same meaning as in fig. 1. The straight line represents the leading term of the asymptotic long time behavior up to second order in c. The error bars are also indicated.

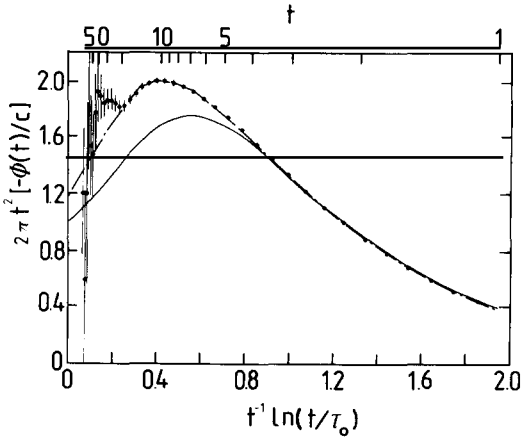

Fig. 3. VACF times t^2 as a function of $t^{-1}\ln(t/\tau_0)$. The curves and the circles have the same meaning as in the preceding figures.

Finally, the time-dependent diffusion coefficient $D(t)$ has been computed using eq. (9) and the result is shown in fig. 4. The theoretical values are also plotted. As happens with the VACF, the MC data agree with the second order approximation within the statistical error. Notice that, even without knowing any theoretical prediction, an extrapolation to $t^{-1}\to 0$ of our MC data would provide a value for the static diffusion coefficient with an accuracy better than 0.05%.

In conclusion, there is a quite good agreement between kinetic theory and the MC simulation that we present in this note. The results show that, at least for short and moderate times, the concentration expansion up to the second order is sufficient for

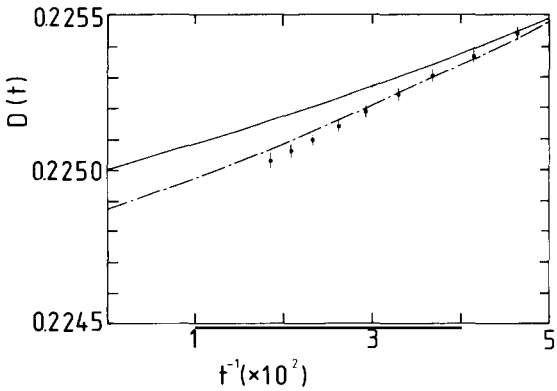

Fig. 4. Time dependent diffusion coefficient as a function of t^{-1}. The meaning of the circles and the curves is the same as in the preceding figures.

$c=0.05$. This indicates that the convergence of such an expansion is not very slow. Nevertheless, the verification of the long time tail of the VACF is only indirect, since if one tries to clearly identify its amplitude, the required computer time seems to be beyond the present computer availabilities, even in these very simple models.

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