SIMULATION RESULTS FOR THE VELOCITY AUTOCORRELATION FUNCTION IN A BOND PERCOLATION MODEL

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Computer simulation results for the velocity autocorrelation function in a two-dimensional bond percolation model are presented, both below and above threshold. Comparison with the effective medium approximation shows an excellent agreement for short and intermediate times, whereas significant discrepancies appear in the long-time region.

The theoretical calculation of the velocity autocorrelation function (VACF) for all times is a quite difficult problem in statistical mechanics. Recently, a great deal of work has been devoted to the study of this quantity in disordered lattices. For low concentrations of defects, methods of kinetic theory have been applied and exact results have been obtained [1]. Exact results for higher concentrations are only available in the short-time limit [1]. Beyond the above limits, approximate methods have been introduced (see e.g. ref. [2]).

Here, we will deal with one of the most extensively studied models, namely the so-called bond percolation model. This is a kind of Lorentz system where independent random walkers move in a lattice having a concentration c of missing bonds. The system exhibits a percolation threshold at a given concentration c_0. In the following, we will restrict ourselves to a two-dimensional lattice, for which $c_0=0.5$. The (exact) short-time behavior of the VACF $\Phi(t)$ in this model is [3]

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

where the edge of the unit cell and the inverse of the jump frequency have been taken as units of length and time, respectively.

Ernst and co-workers [4] have calculated the VACF for all times in the effective medium approximation [5], $\Phi_{\mathrm{EMA}}(t)$. Their results agree with the exact asymptotic behavior given by eq. (1). Also, $\Phi_{\mathrm{EMA}}(t)$ is exact up to first order in the concentration and gives a good approximation for the second order. In addition, the exact value $c_0=0.5$ is obtained. Another prediction of the EMA is that the asymptotic long-time behavior of the VACF above threshold ($c<c_0$) is given by

$$\Phi_{\mathrm{EMA}}(t)\approx -\frac{1-\epsilon}{4\pi\epsilon t^2[1+(4/\pi\epsilon^2 t)\ln(t/\tau)]}\,, \qquad (2)$$

where $\epsilon=1-c/c_0$ and

$$\tau=(1/8\epsilon)\exp[-\tfrac{1}{4}\epsilon(\pi+2)+2-\gamma_{\mathrm{E}}]\,, \qquad (3)$$

γ_{E} being Euler's constant. Eq. (2) shows a t^{-2}-long tail, that is characteristic of two-dimensional Lorentz models [6].

The above facts lead Ernst et al. to expect the EMA to be a reasonable approximation over the whole parameter space. The aim of this Letter is to present some computer simulation results for the VACF and compare them with the EMA. To the best of our knowledge, previous comparisons have been restricted to the diffusion coefficients [2,5]. We have considered concentrations beyond the low density region, namely $c=0.2$ and 0.3 (above threshold) and $c=0.7$ (below threshold). In our study we have not explored the neighborhood of the threshold point, where some interesting features have been analyzed within the EMA [4].

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Although in the theoretical calculations the time is considered as a continuous variable, it is advantageous to use in the simulations a discrete time step [7,8]. In this case, the velocity components can take just the values 0 or ± 1. Also, in order to reduce the statistical errors, the discrete VACF is computed as [7]

$$\Phi_n = \tfrac{1}{2}\langle v_0 \cdot \delta v_n \rangle , \qquad (4)$$

where v_0 is the velocity of the particle at $t=0$, and δv_n is the difference between the actual velocity at $t=n$ and the velocity the particle would have at that time if it moved in an ideal lattice without defects. The angular brackets denote average over both the trajectories and the lattice realizations. Once the Φ_n are known, it is straightforward to obtain the continuous VACF $\Phi(t)$.

For each concentration, we have generated 1320 square lattices of size 700×700 with randomly distributed missing bonds. In each lattice realization the motion of 500 independent walkers has been followed during 1200 time steps. By using the invariance under time translation, each value of Φ_n up to $n=200$ has been obtained by averaging over $N=660\times10^6$ single values. The statistical errors have been estimated by first evaluating the standard deviation $\Delta_{N_1}\Phi(t)$ of the averages corresponding to 22 samples of $N_1=30\times10^6$ values each. Then, by assuming that the error decreases as $N^{-1/2}$, we get $\Delta_N\Phi(t)=\Delta_{N_1}\Phi(t)/\sqrt{22}$. The exact values of the first few discrete Φ_n can be obtained from eq. (1) and the relation between Φ_n and $\Phi(t)$. We have compared the simulation values with the exact ones and found that in all cases the deviation is less than 0.01% for Φ_0, and less than 0.1% for Φ_1 and Φ_2. Besides, these deviations are within the estimated error bars.

The results obtained in the simulation and the EMA predictions for $c=0.2$ and $c=0.3$ are shown in figs. 1 and 2, respectively. Also, the exact short-time behavior given by eq. (1) and the EMA long-time behavior, eq. (2), are plotted. The comparison shows that the EMA is quite a good approximation in both cases up to times of the order of 10. Notice that this range extends far beyond the region correctly described by the exact short-time behavior. For times larger than $t\approx10$, the discrepancies grow rather fast. More precisely, the relative difference between the

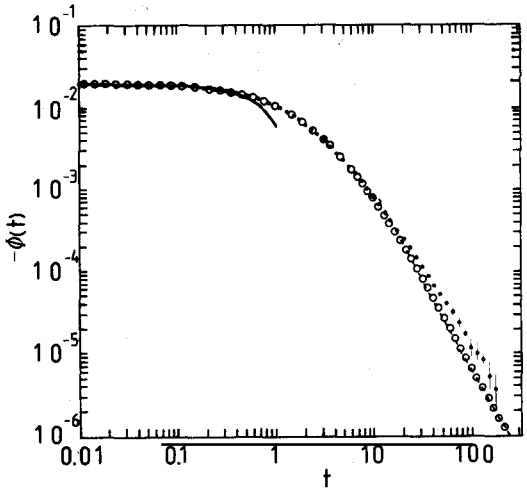

Fig. 1. Log–log plot of the VACF versus time for a concentration $c=0.2$. The dots with error bars are the simulation data and the circles represent the EMA results. The solid line is the exact short-time behavior, given by eq. (1). The broken line is the EMA long-time behavior, given by eq. (2).

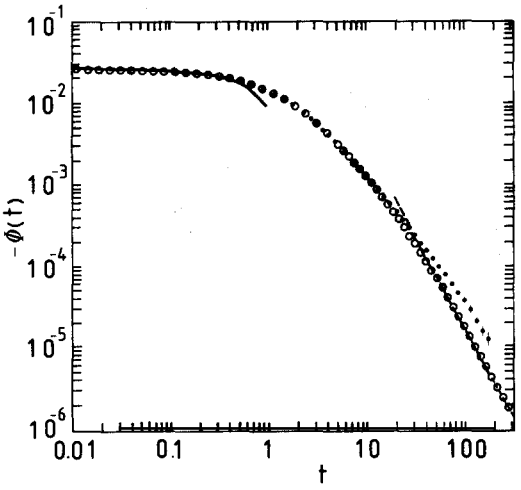

Fig. 2. Same as fig. 1, but for $c=0.3$.

simulation data and the EMA predictions becomes about 20% at $t=20$ for $c=0.2$, and at $t=30$ for $c=0.3$. This result deserves some comments. In principle, since the EMA is exact in the low density limit, one could expect the agreement for $c=0.2$ to extend to larger times than for $c=0.3$. On the other hand, figs. 1 and 2 show that the time region where the differences between the simulation data and the EMA results become relevant coincides approximately with

the region where the latter are accurately described by the long-time behavior given by eq. (2). In other words, the EMA seems to be correct up to the onset of its long time tail, but not beyond. This is consistent with the fact that the agreement region of the EMA with the simulation is larger for $c=0.3$ than for $c=0.2$, since the EMA predicts [4] that the long-time region appears later as the concentration increases towards $c_0=0.5$.

Although the simulation data do not reach times long enough to clearly identify the asymptotic behavior of $\Phi(t)$, it seems evident that this is not correctly described by the EMA, at least at a quantitative level. If one assumes a t^{-2}-tail, this one seems to appear later than predicted by the EMA. In addition, the trend of the simulation points indicates that the amplitude of the tail is rather larger than the one given by eq. (2). If the simulation points in figs. 1 and 2 are fitted to a law of the form $\Phi(t) \sim t^{-\alpha}$, an exponent close to the EMA value $\alpha=2$ is obtained for $c=0.2$, while a smaller exponent is measured for $c=0.3$. This apparently non-universal behavior of the exponent α was first observed in a Lorentz gas by Alder and Alley [9].

A similar comparison for $c=0.7$, that corresponds to a situation below threshold, is presented in fig. 3. Again, there is quite a good agreement for short and intermediate times, whereas significant discrepancies appear for long times. A relative deviation of about 20% is observed at $t=35$, and it grows very fast as time increases. The EMA predicts a long-time decay that is essentially exponential [4], but its explicit expression is not known. Therefore, we cannot check whether in this case the asymptotic region coincides again with the region of discrepancy. The most intriguing feature of fig. 3 is the apparent algebraic tail, which is characteristic of concentrations $c<0.5$, exhibited by the simulation data. This seems to indicate that the system has not yet reached the asymptotic long time behavior. This is consistent with the following physical argument. Consider the picture of the lattice below threshold as composed of finite "islands" with a size distribution that is exponentially cut off. From fig. 2 of ref. [10] we have estimated an average size of islands $\langle N_c \rangle \approx 10$ for $c=0.7$, while in our simulation the mean square displacement is $\langle r^2(t) \rangle \approx 0.7$ for $t=150$. It follows that the times reached in the simulation are not long

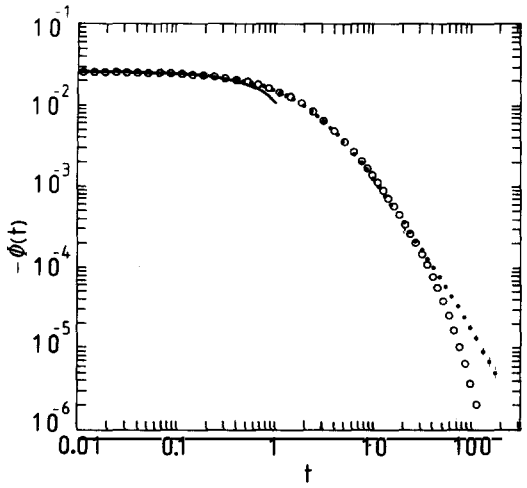

Fig. 3. Same as fig. 1, but for $c=0.7$.

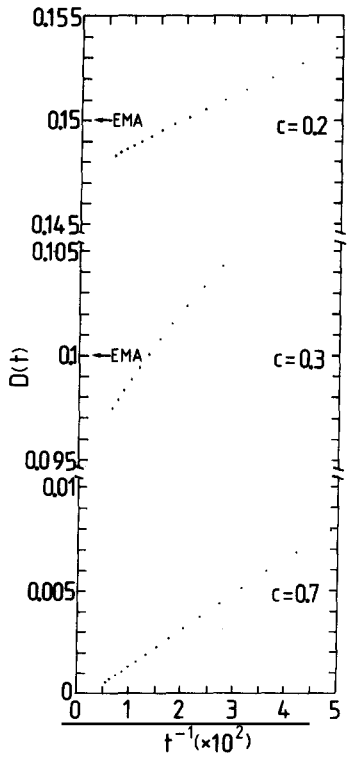

Fig. 4. Simulation values of the diffusion coefficient $D(t)$ for the three concentrations considered. The arrows indicate the locations of the EMA static diffusion coefficient $D_{EMA}(\infty)$, for $c=0.2$ and 0.3.

enough for the random walker to fully realize of the finite size of a typical island.

Finally, the time-dependent diffusion coefficient defined as

$$D(t)=\int_0^t \mathrm{d}s\, \Phi(s) \qquad (5)$$

is plotted in fig. 4 for the three values of the concentration. Also, the EMA values for the static diffusion coefficient $D_{\mathrm{EMA}}(\infty)=\frac{1}{4}(1-2c)$ are shown for the cases above threshold. Extrapolation of the simulation data to $t^{-1}\to 0$ leads to estimated values of $D(\infty)$ that are slightly below the EMA ones. The difference is about 1.5% for $c=0.2$ and about 5% for $c=0.3$. The t^{-1}-behavior of $D(t)$ for $c=0.7$ shown in fig. 4 is again indicative that regular diffusion takes place for the considered range of time. However, an effective static diffusion coefficient for those intermediate times is not reached because the motion of the random walker is strongly inhibited by the high concentration of missing bonds. In fact, an extrapolation of the data for $c=0.7$ to $t^{-1}\to 0$ yields an unphysical negative value. Since $D(t)$ must tend to zero as time goes to infinity, a crossover in the behavior of $D(t)$ is expected for times much longer than the ones reached in the simulation.

In conclusion, the EMA is an excellent approximation for the VACF in the short and intermediate time regions both below and above threshold, but not when the long-time behavior is considered. It must be noticed that the agreement of the VACF is a much stronger test than that of the diffusion coefficient or the mean square displacement.

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