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Random surface deposition of diffusing dimers in two dimensions

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Abstract

Random sequential deposition of diffusing dimers onto a two-dimensional lattice is investigated by Monte Carlo simulation. We find that the jamming occupation for the static case is surpassed; however, the completely filled state is not reached due to the appearance of "dynamically jammed structures". The conjectured time dependence law $(1/t)\ln t$ for the hole population fails to fit the simulations.

Lattice gas models have raised considerable interest due to their multiple applications in physical and chemical processes. The inclusion of random sequential deposition (RSD) has broadened their scope making them capable of modeling reactions on polymer chains, chemisorption on single crystal surfaces, adsorption in colloidal systems, biological growth and spreading, thin film formation and coating, and many other systems as well. These applications have been reviewed by Evans [1]. Deposition with diffusion has received attention recently. Dimers in 1-D [2,3] and hard squares in 2-D [4,5] have been studied, and the subject has been reviewed by Privman [6].

It is well known [1] that in irreversible (i.e. without diffusion) RSD, jamming occurs at an occupation which depends on the number of dimensions and on the animal being deposited. For the case of dimers in 2-D, the critical occupation is $\theta_c = 0.9068$. The source of this jamming is that isolated vacancies arise easily through random deposition. However, when diffusion is allowed, it becomes possible for isolated vacancies to come together and create a site apt for an animal to occupy. The question arises whether or not the diffusion of the animals (or, alternatively, of holes) leads to total occupation.

In this study, we address this question for the case of dimers in 2-D. Though it has been said that diffusion may allow the system to reach a completely filled adsorbed state [3], we find that this turns out to be true only for the 1-D case, for in 2-D the appearance of "dynamically jammed structures" during the filling process prevents the lattice from reaching such a state.

We performed Monte Carlo (MC) simulations of RSD of diffusing dimers in $L \times L$ square lattices with periodic boundary conditions at several values of L and of the incoming dimer flux (f).

The simulation is carried out as follows: in each MC step, $L^2 f$ dimer depositions are attempted. This is

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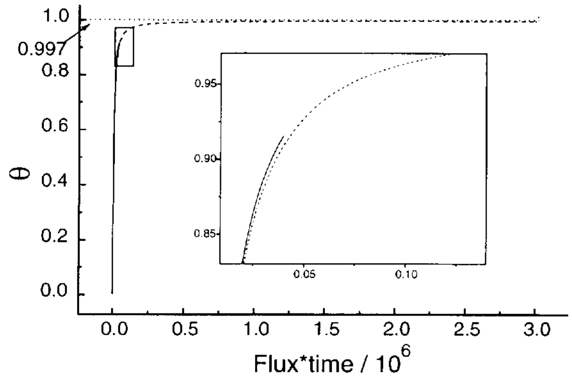

Fig. 1. Occupation versus ft. (—) $f = 0.001$, (- - -) $f = 0.1$.

done by randomly choosing a site, then an orientation (horizontal or vertical) with equal probability. If both sites are empty, the dimer is deposited. Then, for as many times as the number of dimers already deposited, a dimer is picked at random and diffusion or rotation (with equal probability) is attempted. This way, in each MC step $L^2 f$ depositions are attempted and each deposited particle attempts one jump in the mean.

As a detailed description of dimer diffusion on a two-dimensional surface is given elsewhere [7] we give here only a brief sketch. Two possible mechanisms are allowed: the "straight through" (diffusion) mode, in which the dimer moves one site through its axis direction, and the "swing" (rotation) mode in which one of the atoms remains fixed and the other swings 90 degrees. Diffusion involves two site-hoppings, while rotation involves only one, thus the energy barrier of the first is twice that of the second. However, while the diffusion requires only one empty site, in a rotation the moving monomer would transiently occupy a second one.

In Fig. 1 we have plotted the lattice occupation θ versus flux $\times$ time for $L = 100$ and $f = 0.001$ and 0.1. It is clear that the jamming occupation for the static case is surpassed. For the times simulated, an occupation of 0.998 is reached.

However, occupation does not reach 100%, for we find that several configurations exist in which isolated holes are trapped, either forced to remain still, or constrained to a path were they cannot meet other holes. Some possibilities are shown in Fig. 2. It should be noted that the jammed configurations are more complex in RSD of dimers than in the case of squares, since holes can be prevented from meeting not only by

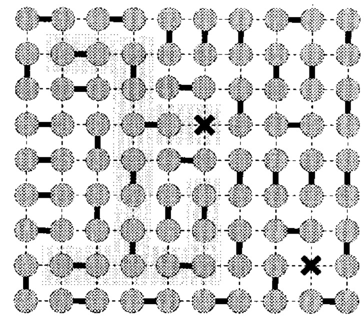

Fig. 2. An example of a dynamically jammed state. One of the holes cannot move at all, while the other can move only within the shaded area. They can never meet to form a site apt for dimer deposition.

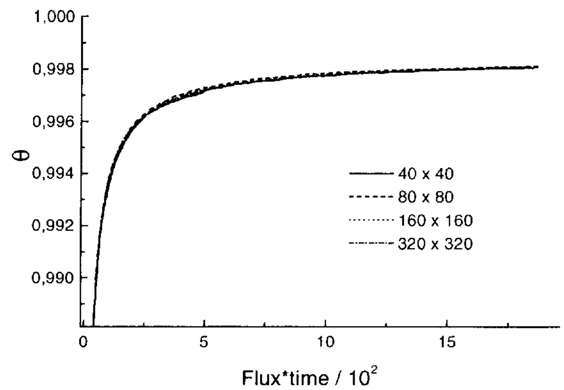

Fig. 3. Occupation versus ft for $f = 0.21$ for different lattice sizes. No lattice-size dependent effect is observed.

freezing them on a site. In a typical configuration at high occupations several holes appear that are trapped in circuits like that shown in the figure, some of them quite long.

To look into possible finite-lattice-size effects we performed the simulations at $f = 0.21$ for lattices of $L = 40$, 80, 160, and 320. We found that the occupation curve was the same in all cases, indicating that dynamically jammed configurations are independent of lattice size (Fig. 3). This is in contrast with the case of 2×2 squares [5], where isolated frozen vacancies develop, but their density at large times goes to 0 for $L \to \infty$, leading in that case to total occupation.

It has been proposed that the hole population should decrease as $(1/t)\ln t$ [1]. This is based on results on diffusion-annihilation reactions [8]. This is not the case; but the approach to the jamming occupation seems to be exponential in time, like in the case of static jamming [6]. The source of the disagreement lies in the existence of dynamically jammed states, which prevent the holes from annihilating. At long times trapping configurations start occurring, and the local anisotropy brought to the lattice by the adsorbed dimers makes the random walk a bad approximation for the motion of the holes.

In conclusion, we find that although diffusion allows coverages greater than the jamming coverage for static dimers to be achieved, dynamically jammed configurations exist which prevent the lattice from being completely covered. Further study is needed to establish the value of the critical occupation in the dynamical case, as well as to accurately describe the time evolution of the occupation θ.

It should be stressed that the kind of defects here observed is different in nature from that described by Wang et al. [4,5] for squares. In the latter case the holes eventually come together (however slowly) and lead to total occupation for $L \to \infty$, $t \to \infty$. For L finite, the jammed configurations have only frozen holes. In the present case, holes appear that can move but are trapped in a closed circuit. This means that jammed configurations can have moving holes (and thus higher entropy). It also helps to explain the observed independence of the θ versus t curves with respect to L, since it shows that jamming arises from local, rather than global, properties of the dimer lattice.

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