DETERMINISTIC LATTICE GAS MODELS

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Two new deterministic lattice versions of the wind-tree model, with fixed or moving mirrors placed randomly on a square lattice are considered. In both cases, the diffusion coefficient apppears to be given by the Boltzmann expression for all densities of the mirrors.

Two lattice versions of the continuous wind-tree model [1,2] are considered, that possess deterministic dynamics of particles between randomly placed scatterers on a square lattice. In these models, a (wind) particle moves on the lattice with initially one of four possible velocities, of magnitude 1 in the $\pm x$- or $\pm y$-direction. Steps of unit length are taken per unit time, carrying the particle one lattice site forward in the direction of its velocity. When the particle moves to a position on the lattice, where a scatterer (tree) resides, it continues to move in a direction perpendicular to its original direction, as if it had hit a mirror positioned at a $\pi/4$- or $3\pi/4$-angle to its direction of motion. In both models, the scatterers are randomly placed on the lattice with a fraction f_1 at an angle $\pi/4$ and a fraction f_2 at an angle $3\pi/4$, so that the particle describes a deterministic, but random-like motion on the lattice. In model A, the mirrors are fixed for all time, while in model B, the mirrors flip at collision over an angle $\pi/2$, changing from a $\pi/4$-angle to a $3\pi/4$-angle mirror and vice versa. We studied the diffusion process for both models and we present some results of our computations for the case $f_1=f_2$, carried out by letting an Atari ST 1040 run for about 48 hours. There is an important difference with the deterministic models studied so far in the literature [3,4] in that no time-dependent dynamics is introduced in our models, whereas for some models in refs. [3,4] collision events differ according to whether they occur at even or at odd times.

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The calculations were performed for a square lattice of 360×360 lattice sites. Instead of considering the motion of a single particle, the motions of a small group of 50×50 particles placed initially in the center of the lattice with either parallel or random velocities were followed.

For model A this implies the simultaneous consideration of a number of independently moving particles and a diffusion process under equilibrium conditions, where the diffusion constant will only depend on the concentration of the scatterers. However, for model B, the spatially inhomogeneous initial condition is not an equilibrium condition and the diffusion coefficient will depend, in principle, on the concentration of the scatterers as well as the particles, since both determine the amount of flipping of the mirrors.

In the case of parallel initial velocities, a random velocity distribution was observed after a few collisions. Subsequently, a much slower approach to a diffusion regime followed, where the mean square displacement of the particles $\Delta(t)$ approached a behavior like $4DT$ with a diffusion constant D, which is independent of the time t. The characteristic time to reach a level of about ninety percent of the final diffusion constant was of the order of ten collision times. This time was found to be independent of the density of the scatterers and the same for fixed and flipping mirrors. It was short compared to the time needed to get a one percent accuracy of the diffusion constant, which took much longer for model A than for model B.

For each density and for both models we let the system of 2500 particles, starting in a central square on a 360×360 lattice, run for 700 time steps. Although we used periodic boundary conditions, the mean square displacement of each particle crossing a boundary was calculated as if it had entered a neighboring replica of the original square.

Although there are important differences between the two models as to the occurrence of closed orbits, the diffusion constant D appears to be the *same* for *both* models, for *all* densities of the mirrors considered, i.e., $0.1 \leqslant f \leqslant 1$, where $f = f_1 + f_2$. Within the present accuracy of the calculations, the value of D could be represented by the Boltzmann value [3,4] (cf. fig. 1):

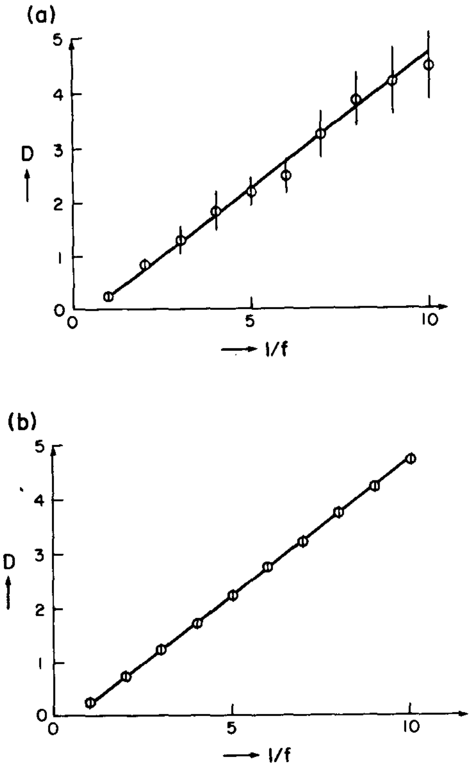

Fig. 1. The diffusion coefficient D as a function of the inverse density of scatterers $1/f$ for model A (a) and model B (b), with error bars.

$$D_{\mathrm{B}} = 1/2f - \tfrac{1}{4} . \qquad (1)$$

A least squares fit of the form $D = a/f - b$ actually gave $a = 0.478 \pm 0.04$ and $b = 0.15 \pm 0.17$ for model A and $a = 0.495 \pm 0.006$ and $b = 0.245 \pm 0.025$ for model B.

Since in the Boltzmann theory each collision of a moving particle with a scatterer takes place as if no previous such collision with the same scatterer has occurred, eq. (1) implies that contributions of non-Boltzmann-like orbits, where the particle returns (once or more) to a position it had visited before (which includes closed orbits), was, for the times that we observed the particles, not noticeable. This appears to be consistent with the results of the calculations for other lattice gases, where all particles are allowed to move and where the viscosity of such a lattice gas is, in good approximation, also given by its Boltzmann value [5].

In order to see how the diffusion process is related to the occurrence of closed orbits, we calculated the total number of phase points associated with such orbits. A phase point is given by the position and the velocity of a particle. Since no closed orbits were observed for model B, we only made a histogram for model A. In fig. 2, we divided the horizontal axes into 18 bins of width 2^n, with $n = 0, 1, \dots, 17$. The height of each bin is proportional to $N_n = \sum_l l N_l$, where the summation extends only over orbits with length l in a given interval $2^n \leqslant l < 2^{n+1}$ ($n = 0, 1, \dots, 17$) and N_l is the corresponding number of orbits. The figure refers to a square 190×190 lattice with reflecting boundaries constructed by letting the two kinds of mirrors alternate along the boundary. Each histogram represents the result of the sum over ten runs with ten different (random) mirror configurations at a given density of mirrors. The distribution of periodic orbits as shown in fig. 2 will not be different if we change to periodic boundary conditions. In that case, an orbit must be considered closed as soon as the starting point, either in the original square or in a replica, is reached again. Also in this case the orbit will never be longer than 190×190, because if any part of the orbit has been traversed once, the same part or any of its images will not be covered again before the orbit is closed. This suggests that, as long as most particles have not yet completed a full revolution through the periodic orbit on

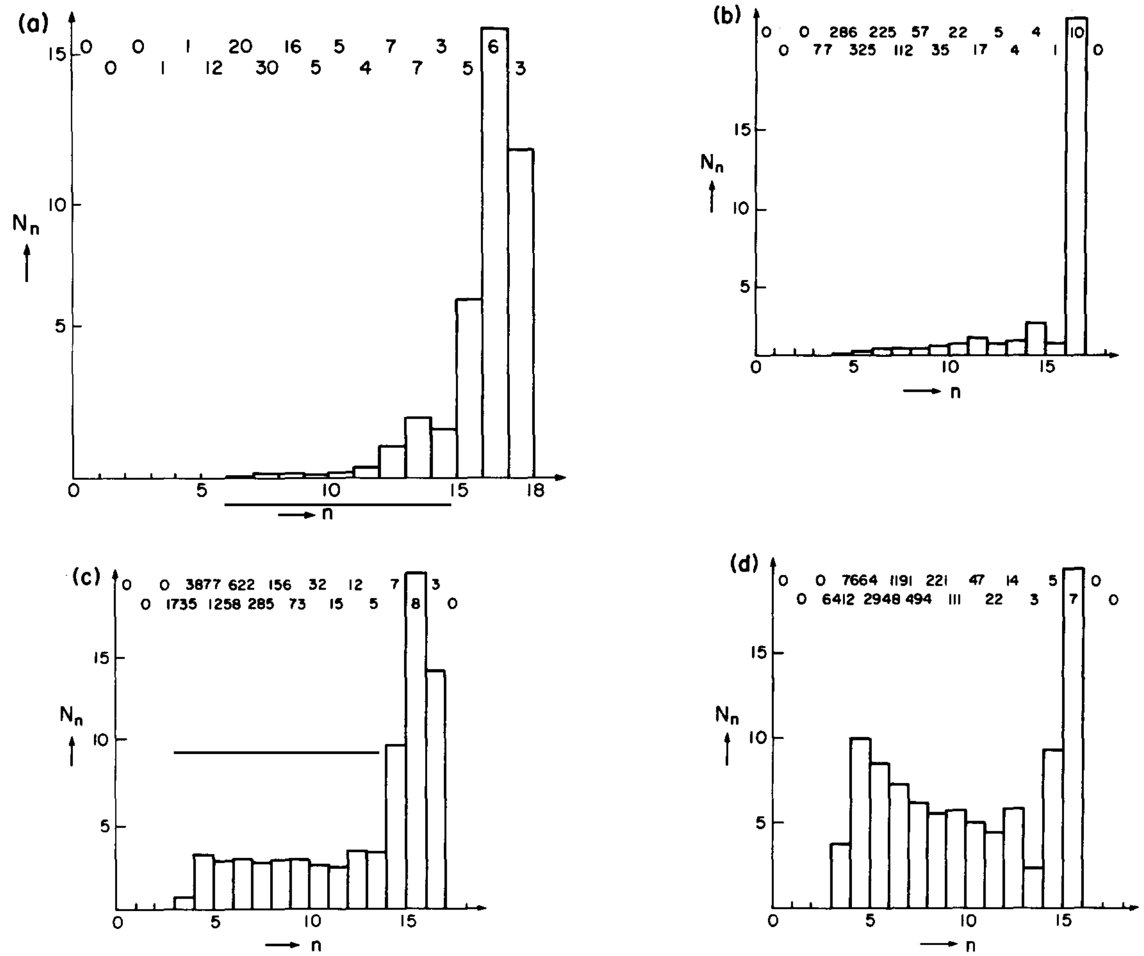

Fig. 2. Distribution of periodic orbits on a 190×190 lattice for reflecting walls after 10 runs. Horizontal axis: N_n is the number of phase points associated with periodic orbits with length in nth bin (arbitrary scale). Numbers above binds: number of periodic orbits in bins. $f=0.1$ (a); $f=0.4$ (b); $f=0.8$ (c); $f=1$ (d).

which they are moving, the diffusion is the same as for an infinite lattice.

We observed that for all but the highest densities, i.e., for $0.010<f<0.80$ most of the phase points belong to only a few but very long orbits, which appear to be responsible for the diffusive behaviour in model A. We note that the distribution of closed orbits for these densities is quite different from that found by Binder [3] for a similar model at a density $f=0.03125$.

Since for low densities the distribution of closed orbits in Binder's model is completely different from the distribution in our model A and since in both models a diffusion process takes place, it appears that the existence of closed orbits does not prevent normal diffusion to occur, at least on the time scale we considered. This obtains even for the highest densities $0.8\leqslant f<1.0$, where in spite of the occurrence of very many closed orbits in model A, diffusion still occurs and moreover with a diffusion constant that is still the same as in model B, where no closed orbits occur.

There are a number of points that could be studied further, apart from the influence of the periodic orbits on the diffusion process. These would include the case $f_1\neq f_2$; the correlations induced between the mirrors in model B, due to collisions with the particles and a comparison with the two-dimensional random walk, especially with varying step lengths.

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