Simulation of Diffusion in a Two-Dimensional Lattice-Gas Cellular Automaton: A Test of Mode-Coupling Theory

D. Frenkel
Fundamenteel Onderzoek der Materie (FOM) Institute for Atomic and Molecular Physics, P.O. Box 41883, 1009 DB Amsterdam, The Netherlands

M. H. Ernst
Institute for Theoretical Physics, P.O. Box 80.006, 3508 TA Utrecht, The Netherlands
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We compute the velocity autocorrelation function of a tagged particle in a two-dimensional lattice-gas cellular automaton using a method that is about a million times more efficient than existing techniques. A t^{-1} algebraic tail in the tagged-particle velocity autocorrelation function is clearly observed. The amplitude of this tail is predicted to within a few percent by a lattice-gas version of mode-coupling theory. The magnitude of logarithmic corrections to the t^{-1} tail is much smaller than expected for continuous fluids.

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Lattice-gas models are ideally suited to serve as a testing ground for concepts in kinetic theory. This is so because the simple structure of lattice-gas models makes it comparatively easy to work out the consequences of a particular approximation scheme in kinetic theory. Such approximations can then be tested numerically, because lattice-gas models are well suited for simulation. In this Letter we present a computational scheme that makes it possible to compute certain transport properties of lattice gases with hitherto unachievable accuracy. Using this technique it is possible to compute the tagged-particle velocity autocorrelation function (VACF) in a simple model for a hydrodynamic fluid, namely a two-dimensional (2D) lattice-gas cellular automaton (LGCA) of order 10^2 to 10^3 collision times, thus enabling us to measure accurately the amplitude of the t^{-1} long-time tail and, for the first time, to estimate an upper bound to the magnitude of logarithmic corrections to it.

Such calculations are of fundamental interest for the following reason: Algebraic long-time tails in the VACF of a tagged particle in an atomic fluid were first reported in a classic paper by Alder and Wainwright.[1] These long-time tails are the consequence of coupling between particle diffusion and shear modes in the fluid. According to mode-coupling theory, the leading term in the long-time tail of the VACF for dimension $D > 2$ is

$$\langle v_x(0)v_x(t)\rangle \approx \frac{D-1}{D}\frac{\langle v_x^2(0)\rangle}{\rho[4\pi(D_0+\nu_0)t]^{D/2}} \equiv \frac{d_0}{t^{D/2}}, \quad (1)$$

where ρ is the number density and D_0 and ν_0 are the "bare" self-diffusion constant and kinematic viscosity, respectively. Ever since the discovery of these hydrodynamic tails, it has been realized that a consistent description of mode-coupling effects in a 2D fluid would result in a long-time tail that decays faster than t^{-1}, because in 2D the constants of self-diffusion and viscosity diverge (see, e.g., Ref. 2). A theoretical estimate for the first correction to the t^{-1} tail in a system of hard disks was given by de Schepper and Ernst.[3] According to Ref. 3, this correction [d_1 in Eq. (2)] is negative and proportional to $\ln(t/t_0)/t$ (where t_0^{-1} is the initial decay rate of the VACF)

$$\langle v_x(0)v_x(t)\rangle \approx d_0/t + d_1\ln(t/t_0)/t + \cdots, \quad (2)$$

for $t/t_0 \gg 1$. Forster, Nelson, and Stephen[4] argued that as $t \to \infty$, the tail should be renormalized to $1/t(\ln t)^{1/2}$.

Thus far it has not been possible to compare these predictions directly with computer simulation data because accurate computation of the VACF for $t/t_0 \gg 1$ requires lengthy simulations on large systems.

The present paper focuses on the properties of two-dimensional LGCA's on a triangular lattice [Frisch-Hasslacher-Pomeau (FHP) model[5,6]]. However, the technique has also been applied to other 2D and 3D lattice-gas models such as the square-lattice Hardy–de Pazzis–Pomeau (HPP) model,[7] and lattice Lorentz gases [see Ref. 8].

In LGCA's the particles are constrained to move along the bonds joining the lattice sites. No two particles can move along the same bond in the same direction. The state of the lattice is completely specified by indicating which links are occupied and which are empty. This implies that lattice-gas particles are indistinguishable.

The time evolution of the system is governed by the following rules: (1) Propagation: all particles move in one time step (for convenience we choose $\Delta t = 1$) from their initial lattice position (say, $\mathbf{r}$) to a new position $\mathbf{r}' = \mathbf{r} + \mathbf{c}_\alpha$, where $\mathbf{c}_\alpha$ is the velocity of species α. (2) Collision: the particles at all sites on the lattice undergo a collision that conserves the total number of particles and the total momentum at each site. Usually, these collision rules are deterministic.

Provided that the lattice has a sufficiently high symmetry (for a discussion, see Ref. 9), the equation that governs the time evolution of the distribution function of such a lattice gas becomes equivalent to the Navier-

Stokes equation for an incompressible fluid if the flow velocity is much less than the speed of sound, and all spatial variations in the system occur on a scale that is large compared to the mean free path of the lattice-gas particles. In this respect LGCA's model atomic fluids.

When attempting to compute the VACF of a particle in a lattice-gas cellular automata, one is immediately confronted with a conceptral problem. As all lattice-gas particles are indistinguishable, the VACF of "a particle" is ill defined. As soon as a particle has collided it is no longer possible to tell which of the outgoing particles is the original particle whose VACF we are attempting to compute. To avoid this problem, the particle under consideration must be labeled differently from the rest (say, a "blue" particle in a sea of "red" particles). Once the collision rules for the red and blue particles have been specified we can compute the VACF of a single tagged particle. Such an approach has been attempted by Boon and Noullez for the FHP model[10] and by Binder and d'Humières for the HPP model.[11] However, this method yields poor statistics (only one tagged particle is permissible) and long-time tails could not be detected. An alternative approach has been followed by Colvin, Ladd, and Alder.[12] These authors were primarily interested in the VACF of a tagged particle in a discretized model of hard hexagons on a lattice, but for the sake of comparison, they also measured the autocorrelation function of the fluid velocity at a lattice site in a 2D LGCA. Colvin, Ladd, and Alder were able to detect a long-time tail in this site VACF. However, the long-time behavior of this site VACF is essentially described by the solution of the diffusion equation for small displacements and is, therefore, from a theoretical point of view, of less interest.

In order to implement our numerical scheme to compute tagged-particle VACF's, we must impose one restriction on the rules of the lattice-gas automaton, namely that the collision rules for a tagged particle with untagged particles result in the occupation of the same output states as in the case of collisions between untagged particles. And, most importantly, the tagged particle has equal probability to be in any of the occupied output states. Hence, for the tagged particle the collision rules are stochastic, although to a "color-blind" observer, the rules appear deterministic. Note also that even in "collisions" that have the same input and output states the tagged particle may still change its state.

The essential feature of these rules is that the average velocity of a tagged particle after a collision at site $\mathbf{r}$ depends only on the (colorless) state at that site. We can thus define for every nonempty site of the lattice the average-post-collisional velocity of a tagged particle at that site,

$$\mathbf{v}_{\mathbf{r}}(t)=\frac{1}{N_{\mathrm{occ}}(\mathbf{r})}\sum_{\alpha=1}^{N_{\mathrm{occ}}(\mathbf{r})}\mathbf{c}_{\alpha}, \tag{3}$$

where $N_{\mathrm{occ}}(\mathbf{r})$ is the total number of particles at site $\mathbf{r}$, and $\mathbf{c}_{\alpha}$ are the velocities corresponding to the occupied links. Note that the site velocity at any lattice site $\mathbf{r}$ changes with every time step.

Let us now compute the VACF, $\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle$, by following the histories of *all* particles that end up at position $\mathbf{r}'$ at time $t=0$. To this end we transport the site velocity $\mathbf{v}_{\mathbf{r}}(0)$ [Eq. (3)] to all "connected" neighboring sites. Site $\mathbf{r}+\mathbf{c}_{\alpha}$ is considered connected to $\mathbf{r}$ if the velocity state $\mathbf{c}_{\alpha}$ at site $\mathbf{r}$ is occupied at the start of the propagation step. Next, we compute the average on every lattice site of these propagated averages. We denote this new set of averages by $\mathbf{v}^{(1)}(\mathbf{r})$. These averages are thereupon propagated to all neighboring sites that are linked at $t=1$ and averaged. This yields the set $\mathbf{v}^{(2)}(\mathbf{r})$. Iterating t times, we obtain at all sites $\mathbf{r}'$ the average $\mathbf{v}^{(t)}(\mathbf{r}')$, which is precisely the average of *all* possible velocities $\mathbf{v}(t=0)$ that a tagged particle that finds itself at site $\mathbf{r}'$ at time t could have had at $t=0$. Simply multiplying this quantity with the instantaneous velocities of the tagged particles that are at site $\mathbf{r}'$ at time t and averaging over all particles yields our estimate for $\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle$.

Note that in order to compute the VACF of a tagged particle, use was made of *all* possible starting positions and trajectories that such a particle could have, compatible with the (deterministic) dynamics of the underlying "uncolored" lattice gas. This greatly improves the statistical accuracy. The only additional averaging is over all possible time origins and over independent initial conditions. The present method is similar in spirit to the exact enumeration method of Ben-Avraham and Havlin[13] for kinetic walks on random lattices. The important difference is that by computing a *moment* of the distribution function rather than the function itself, we gain a factor equal to the number of lattice sites (for more details, see Ref. 8).

Simulations of tagged-particle diffusion were carried out for a 2D lattice-gas model (FHP-III, six speed-one particles, one rest particle, with alternating collision rules for odd and even time steps, see Ref. 6). System sizes of up to 500×500 lattice points were studied at densities d ranging from 0.05 to 0.75 (i.e., 5% to 75% occupancy per velocity state).

Figure 1 shows the velocity autocorrelation function of a tagged particles in the 2D lattice gas at a density $d=0.75$. The VACF has been normalized to one at $t=0$. Here, and in all other cases shown, correlations were only computed for time intervals less than the shortest time in which any particle could cross the periodic box. In many of our calculations the statistical error is of order 10^{-6}, which is about a factor 10^3 lower than has been achieved with conventional techniques. Note that such an error reduction corresponds to a gain of 10^6 in computer time.

Initially the decay of the VACF is approximately exponential. The characteristic decay time t_0 of this exponential ranges from 5.6 at $d=0.05$ to 0.33 at $d=0.75$. There is a surprisingly large time interval where the decay is no longer exponential but not yet algebraic. How-

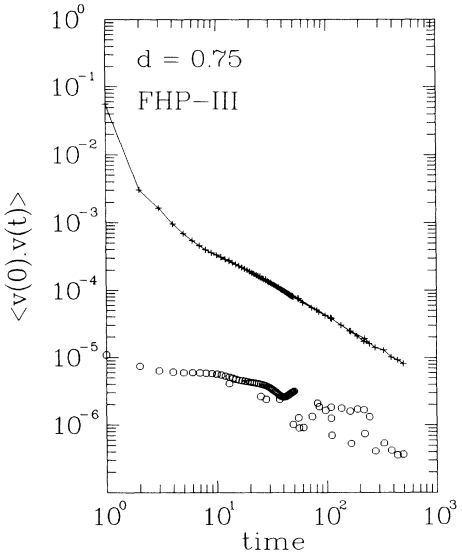

FIG. 1. Example of the normalized velocity autocorrelation function of a tagged particle in a 2D lattice-gas cellular automaton (FHP-III) at a density of 75%. Note that after an initial rapid decay (and overshoot), the VACF approaches a power-law decay with an exponent -1. The estimated error (open circles) decreases with increasing t to a value of order 10^{-6}. In Ref. 10 the statistical error in the long-time tail was of order 0.3×10^{-2}.

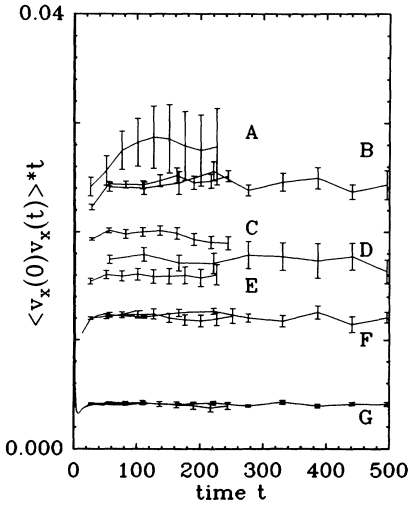

FIG. 2. In order to detect possible deviations from the t^{-1} decay in the VACF of a tagged particle in a 2D LGCA at long times, this figure shows $t\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle/\langle v^2\rangle$ as a function of time t. The letters refer to the density: A-G correspond to $d=0.1$, 0.2, 0.3, 0.35, 0.4, 0.5, and 0.75. For some densities more than one simulation result is plotted. Within the statistical accuracy of the present calculations (the error bars have a length of 2 standard deviations) no systematic deviations from the t^{-1} decay can be detected. However, the error estimate in Eq. (5) is probably too conservative because a fit to the simulation data shows that for all seven points with $d\geq0.3$ the VACF decays with an effective exponent $\beta>1$ (up to 3%).

ever, after some thirty collision times the decay appears to become algebraic. In order to see this latter effect more clearly, Fig. 2 shows the function $t\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle$ for densities $0.1\leq d\leq0.75$. If the VACF decays as t^{-1} then the curves in Fig. 2 should approach a constant value as $t\rightarrow\infty$. Such behavior is indeed observed. This in itself is maybe not surprising, but it is reassuring as it has been argued that the hydrodynamic long-time tails observed in computer simulation on continuous systems may be due to a propagation of numberical errors.[14] In the present simulation the discrete dynamics of the lattice gas is solved exactly, hence propagation of numerical errors is ruled out as a factor affecting either the power-law tails or, for that matter, any corrections to the latter.

We have compared the measured amplitude of the t^{-1} tail with the predictions of mode-coupling theory[15] adapted to the LGCA. As it turns out, the expression for the amplitude of the t^{-1} tail in a 2D LGCA is equal to Eq. (1) multiplied by a factor $1-d$, where the density ρ for continuous fluids must be interpreted as $7d/v_0$, the number density per unit area for the FHP-III model (seven velocity states per site, volume of the unit cell of the triangular lattice $v_0=\sqrt{3}/2$). The factor $1-d$ is a consequence of the Fermi statistics and guarantees that the state occupied by the tagged particle contains no fluid particle. It should be stressed that the applicability of Eq. (1) to the FHP model is not self-evident because in the FHP model there exist unphysical hydrodynamic modes (associated with the staggered momentum density, see Ref. 16). These modes can couple to the microscopic stress tensor, thereby affecting the amplitude of the long-time tail of the stress-stress autocorrelation function. However, to leading order in $1/t$ the same staggered modes do *not* couple to the tagged-particle current.

In Fig. 3 we compare the simulation results for the amplitude of the d_0 with the predictions of mode-

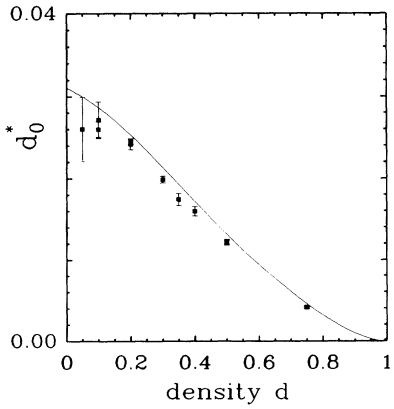

FIG. 3. Density dependence of the amplitude of the t^{-1} algebraic tail of the tagged-particle VACF. Points, computer simulation results. Drawn curve, mode-coupling theory.

coupling theory. As can be seen from the figure, the mode-coupling predictions are very close to the simulation results. The remaining discrepancy of a few percent is comparable to that found by Kadanoff, McNamara, and Zanetti.[16]

Next, consider the behavior of $\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle$ for $t/t_0 \gg 1$. Velocity correlations were studied for times up to $t=500$, which corresponds to values of t/t_0 ranging from 10^2 to over 10^3. In this time regime, which has never before been studied numerically, we would expect to observe a $\ln t/t$ correction to the $1/t$ tail similar to the one predicted by de Schepper and Ernst for the hard-disk model.[3] The relative importance of these logarithmic corrections is grown linearly with the gas density in continuous fluids. If we would assume that the expression for d_1 [see Eq. (2)] given in Ref. 3 also applies in the case of a lattice gas, then we find the following density dependence of the ratio d_1/d_0:

$$d_1/d_0 = -d_0\{(\nu_0+D_0)^{-1}+(4\nu_0)^{-1}+[8(\nu_0+\zeta_0)]^{-1}\} = -0.247d\,, \quad (4)$$

where ζ_0 is the bulk viscosity and $\rho\zeta_0=\frac{1}{14}$ for $\rho=0$.[6] A ratio d_1/d_0 of this magnitude should be easily observable in the present simulations. However, as can be seen from Fig. 2 there is no clear evidence for faster than t^{-1} decay at any density. In fact, a log-log fit to the long-time tail of the VACF allows us to estimate the ratio d_1/d_0 as a function of density. If we assume a linear density dependence of d_1/d_0, we can put the following bounds on the amplitude of this term:

$$d_1/d_0 = -0.02(3)d\,. \quad (5)$$

The kinetic-theory estimate for continuous fluids exceeds this value by 7 standard deviations. This suggests that the expression for d_1/d_0 given in Ref. 3 does not apply to lattice gases. It seems unlikely that the discrepancy is due to the fact that the simulations do not extend to long enough times. More likely, Eq. (4) is not correct for lattice gases, because the density effects of the Fermi statistics have not been accounted for and the staggered momentum modes that do not contribute to d_0 are expected to affect d_1. It should be added that even though we compute $\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle$ for 10^2–10^3 mean free times, we are still well removed from the asymptotic regime where the correlation functions are expected to decay as $1/t(\ln t)^{1/2}$.

At present, the lattice-gas equivalent of the prediction for d_1/d_0 given in Ref. 3 is still lacking. Clearly, such a theoretical result is highly desirable, as it would allow us to decide whether the suppression of significant corrections to the t^{-1} tail is peculiar to lattice gases or if it is indicative of the behavior of 2D fluids in general.

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