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Rapid Communications

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Direct measurement of correlation functions in a lattice Lorentz gas

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We report simulations of a two-dimensional ballistic Lorentz gas on a lattice. A moment-propagation technique allows direct measurements of the velocity correlation function and its moments with low relative errors for all times. We observe the predicted t^{-2} algebraic tails in the velocity correlation function at all studied scatterer densities, unlike what has been reported for continuous systems. In the square lattice a fast $[(-1)^t]$ oscillation is observed, consistent with the existence of staggered density modes. For the second-rank tensor correlation function we find an extremely slow approach to the expected t^{-3} tail.

The discovery by computer simulation[1] of algebraic corrections to the velocity autocorrelation function (VACF) of fluid particles signaled the breakdown of the molecular-chaos assumption and is the starting point of modern kinetic theory. Following the seminal work[1] of Alder and Wainwright, kinetic and mode-coupling theories[2] have been developed that do reproduce a number of these algebraic long-time tails essentially quantitatively. In particular, the hydrodynamic long-time tail now seems well understood.[3] However, significant discrepancies remain for the Lorentz gas,[4] a model where a single particle collides with randomly distributed fixed scatterers. For the Lorentz gas, kinetic theory predicts that the VACF $\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle$ decays as $t^{-(d/2)-1}$ for a d-dimensional system.[5] However, the best simulations to date[6] show an algebraic exponent which in two dimensions varies from -2 to -1.5 as the scatterer density is increased.

There are at least two possible causes for this discrepancy. One is that the simulations may not have probed the truly asymptotic behavior of the VACF, but rather the intermediate-time behavior. There are, in fact, theoretical predictions[7] that the decay of the VACF at intermediate times is apparently algebraic, but with a nonuniversal exponent. Usually the Lorentz-gas VACF has only one negative minimum at short times, but oscillatory behavior and even multiple zero crossings have been observed in certain cases.[8]

An alternative explanation has been suggested in analogy with a phenomenon observed in the study of random walks on a lattice with randomly excluded bonds.[9] In the latter model a crossover to one-dimensional behavior is seen near the percolation point. This reflects a constraint of the available physical space. The value of the high-density exponent observed by Alder and Alley[6] in their study of the "atomic" Lorentz model—with circular scatterers in continuous space—is consistent with this explanation.

In this Rapid Communication we report a numerical study of two-dimensional (2D) Lorentz models in a lattice. Neither of the causes for disagreement between theory and simulation explained in the previous paragraphs is present in these models. We use an accurate, efficient method for the direct calculation of the correlation function of moments of the single-particle velocity. This allows us to perform measurements for up to 900 mean free times at the higher densities, in a model without excluded volume. Only the VACF $\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle$ and the second-rank tensor correlation function (TCF) $\langle 2[\mathbf{v}(0)\cdot\mathbf{v}(t)]^2-1\rangle$ will be considered here.

The main results are as follows: In the square lattice, odd-even oscillations of the VACF are observed, with stronger amplitude at higher scatterer concentrations (c). Both the odd and the even time asymptotes behave as t^{-2}. In the better-behaved triangular-lattice models the strong oscillations are absent and a t^{-2} tail is observed at all studied densities $0.2 \le c \le 0.9$. For these densities, the onset of long-time algebraic tails for the VACF occurs between 24 and 60 mean free times. Figure 2 shows that the approach to this asymptote is by no means monotonic. For the TCF, onset times seem to be even longer, on the order of hundreds of mean free times.

In the model studied here, a particle (or, equivalently, a collection of noninteracting particles), moves at integer time steps from a node in one of the regular space-filling lattices to one of the nearest-neighbor nodes. The particle will move along a straight line until it encounters a scatterer (placed randomly at the nodes with probability

c). During a scattering event in the square-lattice models, the velocity of the particle is either unchanged (probability α), reversed (probability β), or rotated over $\pm\pi/2$ (probability γ), with $\alpha+\beta+2\gamma=1$. Similar rules can be defined in the triangular lattice.

This family of models has been studied theoretically in considerable detail. In particular, a study of the diffusion coefficient is reported in Refs. 10–12, while predictions for the VACF are given in Ref. 13. Two properties of the model are relevant here: (i) there is no "excluded volume," i.e., the particle is not excluded from sites occupied by scatterers. There are, therefore, no physical constraints to the particle's phase space, not even beyond the percolation density of scatterers. (ii) The square lattice can be decomposed into two staggered sublattices, those for which the sum of the x and y coordinates is even and odd, respectively. The particles in this model must go from one sublattice to the other at consecutive time steps. Therefore $(-1)^t$ times the difference of particles between sublattices is a global invariant.[12,14] We shall refer to this invariant as the staggered density. Note that this quantity does not exist in the 2D triangular lattice.

While preliminary measurements of the VACF for the square-lattice model[15] showed deviations from the Boltzmann-level theory for $\gamma\neq\frac{1}{2}$, recent developments of the moment-propagation (MP) technique[3] now allow very precise measurements of long-time tails in lattice systems with stochastic collisions.

The technique consists of propagating not individual particles but moments of the single-particle distribution function on a lattice with (randomly) placed scatterers. It is similar in spirit to earlier techniques that have been used to compute the time evolution of the single-particle distribution function itself (see Ref. 16). However, by focusing on the time evolution of one (or a few) moments of the single-particle distribution function rather than on that of the complete distribution function, a big gain is made in the statistical accuracy with which the moments of interest can be computed. The MP method has been applied to two- and three-dimensional lattice-gas cellular automata[3] and hopping transport on lattices[17] is described in detail in the paper by van der Hoef and Frenkel.[3] The main advantage is that it takes an average over all trajectories consistent with the model and the scatterer configuration, and the relative error remains more or less constant for all times with little increase in computation. This allows for very accurate measurement of the long-time tails at all but the lowest ($c<0.2$) densities of scatterers.[18] The simulations reported in this Rapid Communication were performed on lattices of 256×256 sites (and, in some cases, 512×512 sites). In all cases, correlations were only computed for times short enough that the probability to diffuse over a distance comparable to the linear system size is negligible.

Below we present typical results. Figure 1 is a measurement of the VACF for the square-lattice Lorentz model with isotropic rules, $\alpha=\beta=\gamma=\frac{1}{4}$ at $c=0.9$. Results for other (anisotropic) scattering rules are similar, and will be presented elsewhere.[19] The lower curve provides an estimate of the statistical error in our simulations. Notice the strong oscillations in the VACF for long times. In fact, if we make separate fits for the odd and even values of the VACF to a power series in $1/t$, we find that the coefficient of the leading $(1/t^2)$ term may differ by as much as a factor of 10. This observation suggests that for the square-lattice ballistic Lorentz gas there is no unique long-time asymptote of the VACF. So far the oscillations, caused by the staggered density mode described above, have not been incorporated in the theory for these models. This model, then, seems inappropriate for comparison with theory, and we will focus on triangular-lattice results instead.

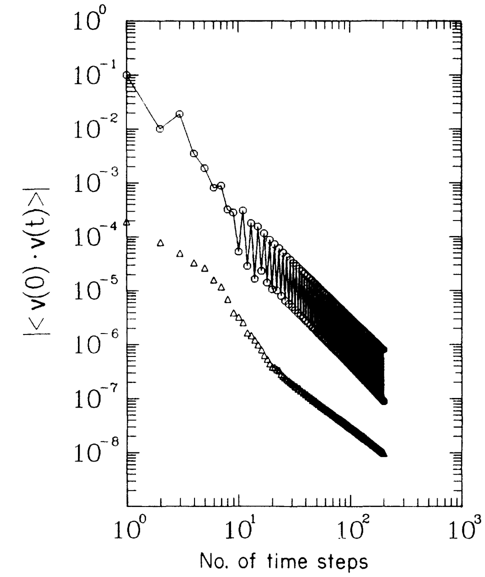

FIG. 1. VACF vs time in the square lattice, isotropic scattering, $c=0.9$. Note the strong oscillations with different asymptotes. The lower curve indicates error bars.

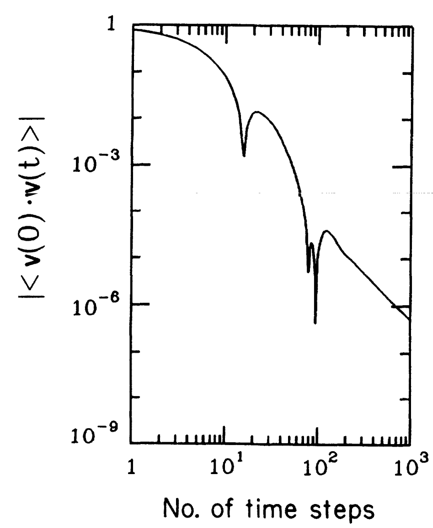

FIG. 2. VACF vs time in the triangular lattice, isotropic scattering, $c=0.2$. Note the peaks (zero crossings). Algebraic tails set in after 300 time steps (60 mean free times).

TABLE I. Amplitude A and effective exponent α of the velocity autocorrelation function of a ballistic Lorentz model on a two-dimensional triangular lattice. The estimated error in the exponent α is shown in parentheses. These coefficients were obtained by fitting the simulation data over a time range $t_{\rm onset} < t < 1000$. The numbers shown in parentheses in the last column are the onset times $t_{\rm onset}$ expressed in mean free times.

c	A	α	$t_{\rm onset}$ ($/t_{\rm mean\ free}$)
0.2	−0.463	2.09(0.22)	300 (60)
0 4	−0.178	2.05(0.05)	90 (36)
0.6	−0.091	2.03(0.03)	50 (30)
0.8	−0.038	2.02(0.03)	30 (24)
0.9	−0.018	2.00(0.02)	30 (27)

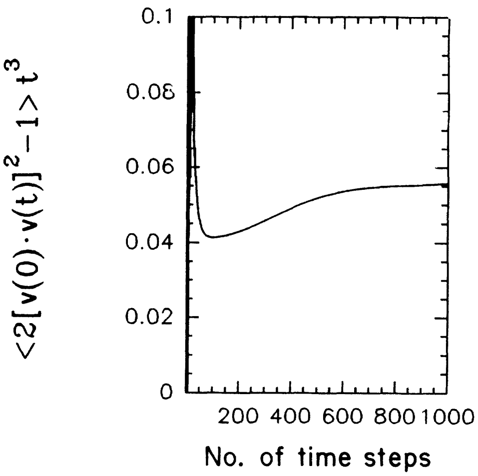

FIG. 3. Stress correlation function multiplied by t^3 vs time, triangular lattice, $c = 0.9$ with isotropic scattering. Notice the very slow approach to a t^{-3} asymptote.

Figure 2 is a measurement of the VACF for the triangular-lattice Lorentz model, also with isotropic scattering rules. The density of scatterers is $c = 0.2$. Note that the long-time oscillations are not present in this case. Also notice the multiple peaks in the logarithm of the VACF: There are zero crossings at $t = 15$, 80, and 95, before the VACF becomes finally negative. The onset of the long-time algebraic tail happens at around $t = 300$, i.e., 60 mean free times. Table I contains a summary of amplitudes, exponents, and onset times for an $At^{-\alpha}$ fit of the VACF for all studied densities. The fits apply to the regime between the onset of long-time tails and $t = 1000$. The fact that there appear to be small systematic deviations from t^{-2} at the lower scatterer densities indicates that the approach to an asymptotic t^{-2} regime, without *any* higher-order terms, will be even slower than indicated in Table I.

Finally, Fig. 3 shows a plot of t^3 times the tensor correlation function versus time for $c = 0.9$ in the triangular lattice. The figure shows that the expected t^{-3} asymptote[13] is approached extremely slowly. In other words, it appears that the amplitudes of higher order (t^{-4}) terms in the TCF are large compared with those of the t^{-3} terms.

In this Rapid Communication we have demonstrated that the VACF of a two-dimensional ballistic-lattice Lorentz model exhibits t^{-2} tails over a wide range of densities, in qualitative agreement with theory. This should be contrasted with the behavior of "atomic" Lorentz gases[6] where the effective exponent of the algebraic tail has been measured to be between -1.5 and -2. At the present we cannot tell whether the crucial difference between our simulations and those on continuous systems is the appreciable difference in the length of the simulations, or the absence of excluded volume effects in the lattice-gas model. We plan to resolve this question by performing simulations on a ballistic Lorentz model *with* excluded volume effects.

In addition, we have shown that the presence of conserved staggered density modes in the square-lattice Lorentz gas models is directly reflected in the presence of strong odd-even oscillations in the VACF.

A final remark is that the intermediate-time behavior is surprisingly rich. It would be interesting to know whether similar intermediate-time behavior is exhibited by continuous Lorentz models. Unfortunately, the existing simulations of the latter models[6] do not extend to long enough times to settle this point.

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[18]P. Scheunders and J. Naudts [Phys. Rev. A **41**, 3415 (1990)], use a similar technique to reconstruct the VACF from two moments of the distribution of times spent by the particle between collisions. Their measurements are consistent with a t^{-2} tail for the studied density range in the isotropic square-lattice model. However, their analysis does not allow them to observe either the fast oscillations or the entire intermediate-time behavior.

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