EUROPHYSICS LETTERS 1 September 1992

Europhys. Lett., 20 (1), pp. 7-12 (1992)

Evidence for Universal Asymptotic Decay of Velocity Fluctuations in Lorentz Gases.

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(received 16 March 1992; accepted in final form 4 July 1992)

PACS. 05.20D – Kinetic theory.
PACS. 51.10 – Kinetic and transport theory.
PACS. 61.20J – Computer simulation of static and dynamic behaviour.

Abstract. – We report a numerical study of the velocity autocorrelation function (VACF) in a lattice model of a Lorentz gas with scatterers that have a finite excluded volume. We observe that, at scatterer densities below the percolation threshold, the VACF decays as t^{-2}. As the percolation density is approached, the onset of the asymptotic t^{-2}-decay shifts to increasingly longer times but the asymptotic exponent itself remains unaffected. Such behaviour appears to contrast with that of off-lattice Lorentz-gas simulations, where the asymptotic exponent was found to vary strongly with scatterer density. Our findings are, however, consistent with percolation-related crossover scenarios proposed by Götze *et al.* (*Phys. Rev. A*, 23 (1981) 2634) and van Velzen *et al.* (*Physica A*, 154 (1988) 34).

The seminal work of Alder and Wainwright [1] has demonstrated that the velocity autocorrelation function (VACF), $\phi(t)$, of a tagged particle in a fluid decays algebraically with an exponent that depends only on the dimensionality d of the system: $\phi(t) \sim t^{-d/2}$. This long-time tail in the VACF is well understood theoretically [2, 3]. In fact, recent simulations of d-dimensional lattice-gas models for simple fluids show that both the amplitude and the exponent of this «hydrodynamic» long-time tail are in essentially quantitative agreement with the theoretical predictions [4]. In addition to the «hydrodynamic» long-time tail in the VACF of a particle in a hydrodynamic fluid, algebraic decay of the VACF is also found in a much simpler system, *viz.* a Lorentz gas. In the Lorentz gas, a single particle collides with fixed, infinitely massive scatterers. For such systems, the theory predicts that, as long as the moving particle is not trapped by the scatterers, the VACF should decay asymptotically as $t^{-(d+2)/2}$. Surprisingly, even though the Lorentz gas is in many respects a simpler model than the atomic fluid, simulation [5, 6] and theory [7] have been in serious disagreement during the past twenty years. In particular, extensive calculations by Alder and Alley [6] indicated that, for a two-dimensional Lorentz gas, the exponent that characterizes the algebraic decay of the VACF varied from the expected value of -2 at low densities to a value close to -1.5 at high densities. More recently, however, extensive simulations on a lattice version of a Lorentz gas have been performed [8]. These simulations appear to yield both qualitative and quantitative agreement with the theoretical predictions. In particular, the latter simulations find an asymptotic t^{-2}-decay of the VACF *at all densities*. There is, however, an important difference between the model studied in ref. [8] and the model studied by

Alder and Alley. In the latter model, the scatterers are modelled as hard disks that have a finite excluded volume. In contrast, the scatterers in the lattice model studied in ref. [8] have no excluded volume. This distinction is important, because it has been argued by Götze *et al.* [9] and, more explicitly, by van Velzen *et al.* [10] that, in a model with excluded volume, the onset of the truly asymptotic decay of the VACF shifts to very long times as the percolation density (*i.e.* the density where the diffusion constant vanishes) is approached. In ref. [9] and [10], it is predicted that for intermediate times, the VACF should decay with an effective exponent -1.5, reflecting effectively one-dimensional diffusive behaviour. However, until now, direct evidence for this scenario was lacking. Clearly, our earlier simulations of lattice models without excluded volume (and hence without percolation) could never reveal the predicted crossover effect.

In the present letter, we report simulations of lattice Lorentz models *with* excluded volume. In all simulations of systems below the (bond-) percolation threshold, we invariably find that, asymptotically, the VACF decays as t^{-2}. However, as the percolation threshold is approached from below, the onset of this t^{-2}-behaviour shifts to longer and, eventually, inaccessible times. Below, we briefly describe the (three) models that we have studied and those aspects of the computational procedure that are not standard.

Let us first consider a lattice Lorentz model *without* excluded volume [8]. In such a model, particles move with unit speed along the bonds of a square or triangular ($2D$) lattice. Particles can only change the direction of their velocity when they encounter a scatterer at a lattice point. A feature of this model is that particles can be at the position of a scatterer. Hence, no matter how high the scatterer density, the entire volume is always available to the particles. If all lattice sites are occupied by scatterers, the moving particles undergo a simple random walk. In order to introduce «excluded volume» into such lattice models, we have to modify the earlier models in such a way that the particles cannot occupy certain sites or bonds. We discuss three realizations of such excluded-volume lattice Lorentz gases on a triangular lattice:

Model A. If a scatterer is present at a site, the particle cannot occupy that site. If a particle arrives within one lattice unit of an occupied site, it can scatter to any neighbouring nonoccupied site with equal probability.

Model B. The same as model *A*, except that the particle can only scatter to unoccupied neighbouring sites which are not simultaneously neighbours of the site that caused the scattering. In other words, the particle can only scatter backwards to unoccupied sites.

Model C. In contrast to the previous two models, no lattice sites are excluded in model *C*, but only bonds. The basic scattering objects are triangles. The moving particle cannot travel along the bonds that form the sides of such a triangle. If a particle arrives at one of the vertices of the triangle, it is scattered in the direction of one of the «open» bonds. Schematic drawings of the three models are shown in fig. 1.

We have concentrated on triangular-lattice models in order to eliminate as much as possible the effect of spurious conserved quantities («staggered» invariants) that are typical of the square lattice [8]. Of course, as will be discussed below, it is not possible to completely eliminate all lattice effects on the VACF (such as odd-even oscillations). Model *A* is by far the simplest and most straightforward to simulate. However, it has an undesirable feature that complicates further theoretical analysis, namely that a particle may recollide immediately with the same scatterer (the probability of such a recollision is 40%). Model *B* avoids this problem, but it is less convenient from a computational point of view: the fact that colliding particles always backscatter appears to enhance odd-even oscillations in the VACF. It takes a long time before these transient oscillations have died away and a unique asymptotic tail is reached. Finally, the bond-exclusion model *C* seems a good compromise between the previous two models. The simulation technique consists of propagating moments of particle distributions rather than the particles themselves. This method, which

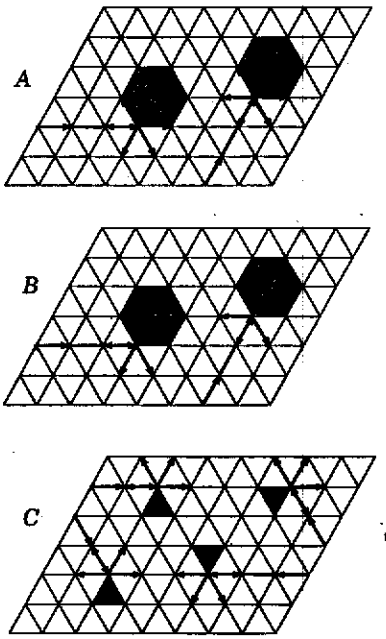

Fig. 1. – Schematic drawing of the three lattice models (*A*, *B* and *C*) that are discussed in this paper. In all three figures we have sketched what happens if an incoming particle hits a scatterer. The colliding particle can scatter in 5, 3 and 4 directions for models *A*, *B* and *C*, respectively. The scatterers are represented as dark hexagons (e.q. triangles).

produces excellent statistics, is analogous to exact enumeration of random walks; it has been described in detail elsewhere [4]. For a given configuration of scatterers, our scheme produces exact results. The only averaging that remains to be performed is over different configurations of scatterers.

In our simulations, we found that it was essential to eliminate the contribution to the VACF due to particles that are trapped in nonpercolating domains on the lattice. At sufficiently long times, such trapped particles yield a small, oscillating, but nondecaying contribution to the VACF that will eventually completely overwhelm the decaying long-time tails of the diffusing particles. To avoid this difficulty, we only follow those particles that move on the percolating (infinite) cluster of sites. In order to identify the largest (percolating) cluster in the system, we have performed a cluster analysis for each configuration of scatterers. As the moving particles in a Lorentz gas only interact with the scatterers, but not with each other, we can perform a simulation in which we simultaneously follow the time evolution of many particles. Initially, we start all particles with the same velocity (say, in the $+x$-direction). The particles are placed on lattice sites that belong to the percolating cluster. Simulations were performed for a range of scatterer densities for each of the three models. In most cases we studied the behaviour of the VACF in the interval $0 \leqslant t \leqslant 1000$ (in units of the basic time step of the lattice gas). For some of the higher concentrations, we computed the VACF for times up to $t = 2000$. Typically, 50 independent configurations of scatterers were generated for each density. In order to eliminate finite-size effects, the linear dimensions of the lattice were chosen to be appreciably larger than the root-mean-square displacement of a particle during the simulation. For most densities, a lattice size of 100×100 sites was found to be adequate. In all cases, periodic boundary conditions were used.

Figures 2-4 show typical results for the VACF for the three models discussed above. In fig. 2,

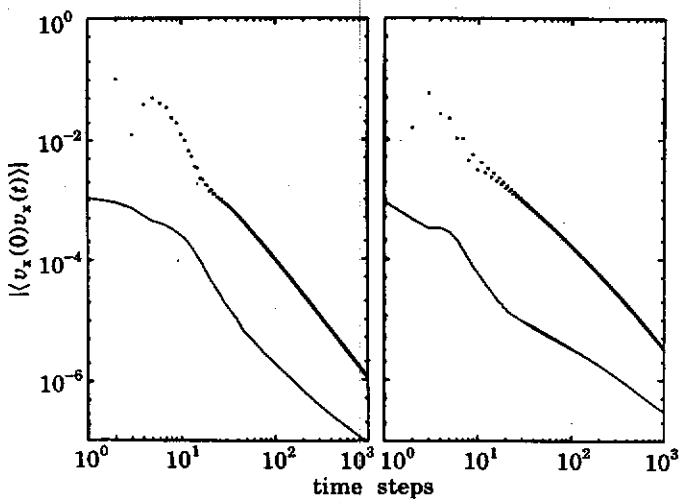

Fig. 2. – Typical VACF measurements for model A. Left: density $d = 0.20$, with long-time tail t^{-2}. Right: $d = 0.35$: the asymptotic algebraic decay is not reached within 1000 time steps. In both figures, the lower curves denote our estimate of the statistical error in the VACF.

we show results for the VACF of model A at two different scatterer densities (a) 20% and b) 35%). Whereas in a) a t^{-2}-tail is clearly visible, in b) the asymptotic behaviour is not reached within the time interval shown. Figure 3 shows a typical result for model B at a scatterer density of 10%. Even-odd effects are visible, as well as slower oscillations which are not yet understood. The tails have barely settled in by 1000 time steps. In fig. 4, we show the VACF for model C at a scatterer density such that 17.5% of the surface is covered by occupied triangles. The VACF exhibits some

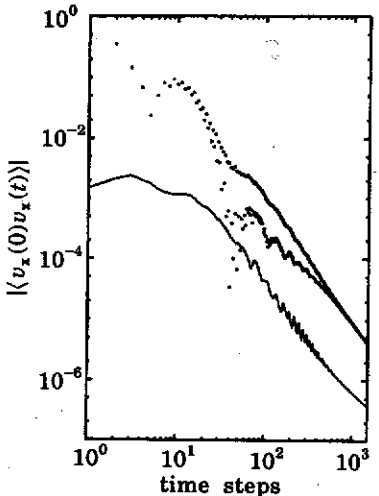

Fig. 3.

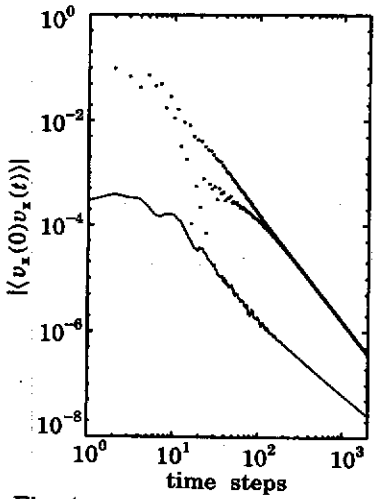

Fig. 4.

Fig. 3. – Typical VACF measurement for model B at a density $d = 0.10$. The t^{-2} long-time tail sets in between 1000 and 2000 time steps. The lower curve denotes our estimate of the statistical error in the VACF.

Fig. 4. – Typical VACF measurement for model C, at a density $d = 0.175$. A t^{-2} long-time tail sets in after $O(10^2)$ time steps. The lower curve denotes our estimate of the statistical error in the VACF.

transient oscillations. However, at longer times a perfectly well-behaved algebraic tail develops. Although we have found algebraic tails in the VACF for all three model systems studied, the onset of the asymptotic behaviour in model B was systematically found to occur much later than in models A and C. We have therefore limited our subsequent analysis to models A and C. The diffusion coefficient D and the amplitude and exponent of the At^{-b}-tails for models A and C are given in tables I and II. We only report those densities for which an algebraic tail has clearly developed within the time window of our simulations. In the same tables, we also list the fraction of sites in the largest cluster. The smaller f, the closer the system is to the percolation threshold. However, as we were not interested in the percolation transition *as such*, we have not attempted to accurately determine the percolation densities for these models. We estimate that the highest densities shown in the tables correspond to some (60 ÷ 70)% of the percolation threshold. For the higher densities, the time at which the algebraic tail sets in is also shown; for lower densities, the times are always below 200 and 700 time steps for models A and C, respectively. The most striking result of our simulations is that, whenever we can observe an algebraic tail at all, this tail decays with an exponent that is, within our statistical errors, equal to -2. As mentioned above, we estimate that we have probed densities up to about 60% of the percolation value. For comparison, Alder and Alley report an exponent of -1.54 for a density value of about half the percolation density.

Our findings are consistent with the scenario in [9, 10], in which there is an exponent crossover very near the percolation threshold. In this scenario, the usual t^{-2}-tails should exist up to the percolation density itself. However, the onset of the asymptotic decay is expected to shift rapidly to longer times as one approaches the percolation density, p_c ($t_{onset} \sim 1/(p_c - p)^2$). At times below t_{onset}, ref. [9, 10] predict that the VACF will decay effectively as $t^{-3/2} \log(t)$. The results of our simulations appear to be consistent with such a percolation crossover scenario. In particular, if we perform a naive algebraic fit of the VACF in the time range $t < t_{onset}$, we find effective exponents

TABLE I. – *Scatterer density d, diffusion coefficient D, amplitude (A) and exponent (b) of algebraic long-time tail, and fraction (f) of sites in the largest cluster for model A. For d ≥ 0.225, t_{onset}, the onset time for the simple algebraic decay, is also shown.*

d	D	A	b	f	t_{onset}
0.075	0.894	− 3.45	2.09 ± 0.13	0.956	—
0.100	0.663	− 1.35	1.95 ± 0.15	0.899	—
0.125	0.489	− 1.05	1.94 ± 0.08	0.874	—
0.150	0.396	− 1.18	1.98 ± 0.06	0.848	—
0.175	0.332	− 0.94	1.96 ± 0.07	0.824	—
0.200	0.297	− 0.97	1.98 ± 0.14	0.799	—
0.225	0.249	− 0.72	1.93 ± 0.07	0.774	200
0.250	0.220	− 0.70	1.91 ± 0.09	0.751	350
0.300	0.173	− 0.89	1.90 ± 0.09	0.700	650

TABLE II. – *Scatterer density d, diffusion coefficient D, amplitude (A) and exponent (b) of algebraic long-time tail, and fraction (f) of sites in the largest cluster for model C. For d ≥ 0.125, t_{onset}, the onset time for the simple algebraic decay, is also shown.*

d	D	A	b	f	t_{onset}
0.050	1.200	− 2.95	2.09 ± 0.11	1.000	–
0.100	0.520	− 1.89	2.07 ± 0.04	0.998	–
0.125	0.384	− 1.29	2.00 ± 0.06	0.995	700
0.150	0.297	− 1.61	2.03 ± 0.05	0.992	800
0.175	0.229	− 1.59	2.01 ± 0.05	0.986	1000
0.250	0.106	− 2.33	1.93 ± 0.10	0.952	1200

b_{eff} that are in between the asymptotic value of -2 and the intermediate-time «percolation» value -1.5 (for example $b_{\text{eff}} = -1.69$ for the VACF shown in fig. 2*b*)). In tables I and II, we also report the amplitude of the asymptotic long-time tail. In principle, these amplitudes can be compared with several theoretical predictions that are either approximate [9, 11, 12], or intractable [12]. Unlike the predictions for the functional form of the asymptotic decay of the VACF, those concerning the density dependence of the amplitude are all rather different both qualitatively and quantitatively. As a comparison of the relative merits of the approximate theories of ref. [9, 11, 12] falls outside the scope of the present letter, we have not attempted to compare our numerical data for the amplitude of the long-time tail with the corresponding theoretical predictions (1).

In summary, in our simulations of excluded-volume lattice Lorentz gases we do *not* find any long-time algebraic tails whose exponent differs significantly from -2. In view of the present results, it seems likely that the discrepancy between the Alder-Alley simulations and the predictions of kinetic theory is only apparent. As the model studied by Alder and Alley has a percolation transition, one should expect that the onset of the asymptotic t^{-2}-decay shifts to longer and longer times as the density is increased. Unfortunately, it is very difficult to measure the VACF for such long times in a continuous Lorentz model. In fact, if time is expressed in units of the mean free time, the current simulations are at least one order of magnitude longer than those of ref. [6]. This difference may explain why in the simulations of ref. [6] the onset of the «universal» t^{-2}-tail was never observed in any but the lowest-density runs.

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We thank M. H. ERNST for many fruitful discussions and M. VAN DER HOEF and B. MULDER for a critical reading of the manuscript. PMB thanks the SERC for financial support, and the FOM Institute for its hospitality. The work of the FOM Institute is part of the scientific program of FOM (Stichting Fundamenteel Onderzoek der Materie) and is supported by the «Nederlandse Organisatie voor Wetenschappelijk Onderzoek» (NWO).

(1) A systematic analysis of this problem in the context of the continuous Lorentz gas has recently been carried out by C. P. Lowe and A. J. Masters, to be published.

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