EUROPHYSICS LETTERS 1 January 1992
Europhys. Lett., **17** (1), pp. 39-43 (1992) *published in November 1991*

Velocity Autocorrelation Function in a Four-Dimensional Lattice Gas.

M. A. VAN DER HOEF, M. DIJKSTRA and D. FRENKEL
F.O.M.-Institute for Atomic and Molecular Physics
Kruislaan 407, 1098 SJ Amsterdam, The Netherlands

(received 22 July 1991; accepted 23 September 1991)

PACS. 61.20J – Computer simulation of static and dynamic behaviour.
PACS. 05.40 – Fluctuation phenomena, random processes, and Brownian motion.
PACS. 05.60 – Transport processes: theory.

Abstract. – We report simulations of the velocity autocorrelation function (VACF) of a tagged particle in a *four*-dimensional lattice gas cellular automaton (LGCA). We observe a hydrodynamic tail in the VACF, which decays as t^{-2}, in agreement with the theoretical predictions. However, in a quantitative comparison, the simulations show that mode-coupling theory underestimates the amplitude of the hydrodynamic tail by $(15 \div 60)\%$. The artificial correlations, previously observed in the projected three-dimensional lattice gas model, are found to be absent in this truly 4D model.

The appearance of hydrodynamic long-time tails in the velocity autocorrelation function (VACF) of a tagged particle in a classical fluid [1] is a phenomenon that is well understood. The physical origin of this long-time tail is that the initial motion of the tagged particle induces a flow field in the fluid, which in turn is responsible for correlations at longer times. A simple dimensional argument [1] indicates that the long-time tail related to such correlations should decay algebraically as $t^{-d/2}$, where d is the dimension of the model-system under consideration ($d > 1$). This prediction is in agreement with observations in molecular dynamics (MD) simulations of two- and three-dimensional systems [1-4]. A more complete description of this long-time tail is given by mode-coupling theory, which takes into account the slow decay of the hydrodynamic modes in the fluid [5], and also by a version of kinetic theory that accounts for the effects of ring collisions [6]. The predictions of these theories are in reasonable agreement with the simulation results mentioned earlier, although such a quantitative comparison proved to be difficult as MD-simulations of long-time tails in three dimensions are extremely time-consuming, and the study of the same phenomenon in four dimensions (4D) is virtually impossible. However, there exists an interesting alternative to molecular dynamics simulations in which the VACF can be measured with extremely high accuracy, namely the study of lattice gas cellular automata (LGCA). LGCA were introduced in 1985 by Frisch *et al.* [7, 8] and can be viewed as molecular dynamics in discrete space and time, or in other words, models in which particles are constrained to move on a lattice. Moreover, particles can only have a few different velocities. As explained in ref. [9], the

VACF can be computed very efficiently in such a system. The simulation results of the VACF in two- and three-dimensional LGCA's have been found to be in essentially quantitative agreement with the prediction of mode-coupling theory [10-14]. The main objective of the present letter is to verify the existence of an algebraic long-time tail in a four-dimensional model fluid and to compare the simulations with the predictions of the corresponding mode-coupling theory. In addition, the present simulations also allow us to gain some more insight into the model that is generally used in three-dimensional lattice gas simulations [15, 16]. This is so because this three-dimensional model is actually a *projection* of the four-dimensional model that is under study in the present letter. The reason why a projected four-dimensional lattice gas is used as a model of a three-dimensional fluid is that there exists no three-dimensional lattice with high enough symmetry to ensure macroscopic isotropy of the equations of motion. One consequence of this projection is that spurious correlations exist in the velocities of different particles. In particular, due to the projection of the 4D lattice, two particles can recollide without colliding with any other particle. These peculiar recollisions manifest themselves in the VACF at short times. The effect is most striking for correlations after two time steps. At that time, recollisions have not yet taken place and hence the VACF of an unprojected model would show Boltzmann behaviour. In contrast, the VACF of the projected model shows deviation from Boltzmann behaviour at two time steps, which has indeed been observed in the simulation results of a three-dimensional lattice gas [12]. One of our objectives in the present letter is to show that these spurious correlations are absent in a truly four-dimensional simulation.

The particular model that we have used is defined on a four-dimensional face-centred hyper-cubic (FCHC) lattice, and is usually referred to as the FCHC-model. For the 4D FCHC-model, mode-coupling theory [11, 14] predicts that the long-time tail of the normalized VACF of a tagged particle is of the following form:

$$\frac{\langle v_x(0)\, v_x(t)\rangle}{\langle v_x^2\rangle} = \frac{1}{256\pi^2}\left(\frac{1-f}{f}\right)\frac{1}{(D+\nu)^2 t^2} = d_0 \frac{1}{t^2}, \tag{1}$$

where f is the density, defined as the average number of particles per link ($0 \leqslant f \leqslant 1$). D and ν are the diffusion coefficient and the kinematic viscosity, respectively. Equation (1) defines d_0, the amplitude of the hydrodynamic tail. In the Boltzmann approximation, D and ν can be calculated explicitly as a function of f. The result for the projected 3D model and the nonprojected 4D model are equivalent, and can be found in ref. [11]. In principle, one should use the true values for D and ν, including the non-Boltzmann contributions. In the studies of three-dimensional lattice gas fluids [11, 12] it has been demonstrated that the latter contributions to the transport coefficients are negligible, as they are less than 1% of the Boltzmann value. It therefore seems justified, in the present comparison, to use the Boltzmann values for D and ν. Indeed, our results for the 4D VACF confirm that the non-Boltzmann corrections to D are very small. Our neglect of non-Boltzmann contributions to ν is less well founded, as the stress correlation function cannot be calculated with sufficient high accuracy. Nevertheless, we have numerical evidence that the stress correlation function of a 4D FCHC lattice gas is, to a very good approximation, exponential. This suggests that, unless the decay of the nonexponential part of the stress correlation function is anomalously slow, the non-Boltzmann contributions to the viscosity are not large enough to account for the quantitative disagreement between theory and simulation reported below.

The simulations were performed on lattices of 30^4 lattice sites. The time intervals over which the VACF was measured were in all cases less than the shortest time in which a particle can cross the periodic box. There remains a finite-size effect related to the finite

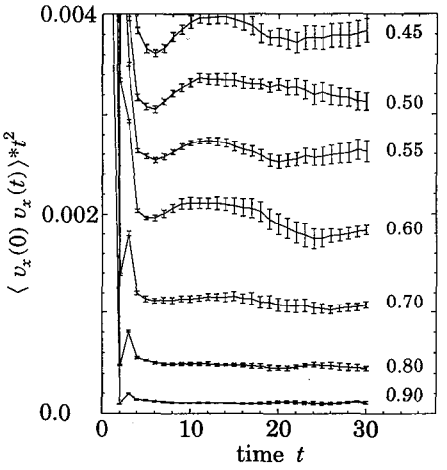

Fig. 1. – Velocity autocorrelation function multiplied by t^2 in a four-dimensional lattice gas. The functions are shown for different densities f, defined as the average number of particle per link. Note that in all cases we observe the expected t^{-2} long-time decay.

number of particles, described extensively in ref. [17]. As discussed in [17], it is straightforward to correct for this finite-size effect. Simulations were performed for different densities varying from $f = 0.45$ to $f = 0.90$. The specific method used to calculate the VACF was the moment propagation method described elsewhere [9, 10]. In what follows we always consider the VACF normalized to one at $t = 0$. In fig. 1 we show the VACF obtained from the simulations, multiplied with t^2, as a function of time. If the VACF decays as t^{-2}, these curves should approach a constant value, as is indeed observed. The values of these plateaus directly represent the tail amplitude d_0, and can be compared with the theoretical prediction. This comparison is shown in fig. 2, where we divided d_0, as obtained from the simulation, by the corresponding theoretical prediction, as a function of f. As can be seen from fig. 2, we find rather large deviations from the theoretical predictions. The theory understimates the amplitude of the long-time tail by some 15% for densities lower than 0.8. For density 0.9 the deviation is about 60%. At present we have no explanation for this

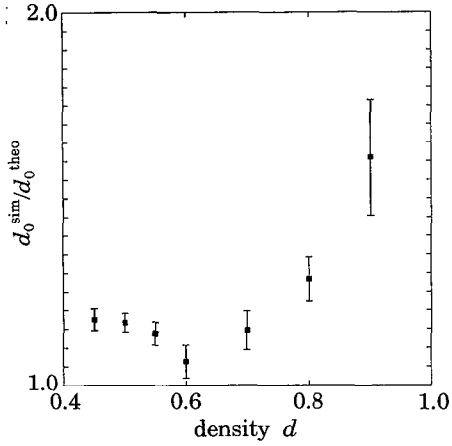

Fig. 2. – Amplitude of the long-time tails (see fig. 1) divided by the theoretical prediction (eq. (1)), as a function of density. Note that at the highest density the deviations from theory amount to 70%.

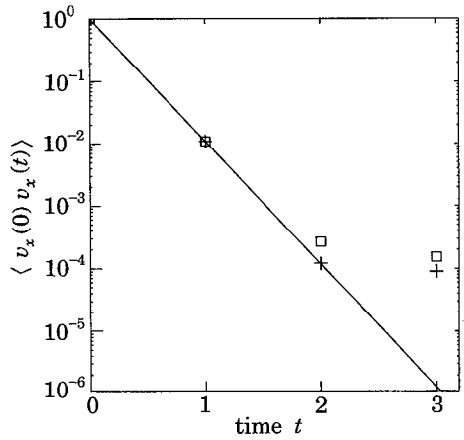

Fig. 3. – Initial decay of the VACF for one particular density ($f = 0.8$) in the 3D and the 4D lattice gas, on a log-linear scale. The simulation data are represented by the «plus» markers (4D model) and the squares (3D model). The error bars on the data points are at least ten times smaller than the size of the markers. The solid line is the prediction in the Boltzmann approximation, for both models, and represent true exponential decay. Note that in the projected 3D model there is deviation from «Boltzmann» after two time steps, which is not found in the true 4D model.

quantitative disagreement. In fig. 3 we show the initial decay of the function on a log-linear scale, for one particular density ($f = 0.8$). In this figure the solid line represents the exact Boltzmann prediction which decays exponentially. The markers indicate the simulation results in the 4D model (pluses), and in the quasi-3D model (squares). We see exponential decay for the 4D model up to 2 time steps, as expected. For the 3D model there is a deviation from Boltzmann-like behaviour one time step earlier. This deviation has been calculated theoretically by Brito and Ernst [18], and was found to be in excellent agreement with our observations. In conclusion, we have observed the hydrodynamic t^{-2}-tail in the 4D VACF. However, there is a surprising quantitative disagreement between the simulation results and the prediction of mode-coupling theory for the asymptotic tail. As discussed earlier, the use of Boltzmann transport coefficients instead of the true Green-Kubo integrands cannot be the cause of this large discrepancy. There are two possible causes remaining. The first is that the usual version of mode-coupling theory is not applicable to 4D fluids in general, which seems rather unlikely. Alternatively, the discrepancy is caused by a peculiarity of the lattice gas model itself. In this context it is natural to think of the many spurious invariants of the 4D FCHC model [19] that may couple to the hydrodynamic modes, and seriously alter the prediction of mode-coupling theory.

* * *

We wish to acknowledge stimulating and useful discussions with M. ERNST and T. NAITOH. We thank A. ALAVI for a critical reading of the manuscript. The work of the FOM-Institute is part of the scientific program of FOM and is supported by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO).

REFERENCES

[1] ALDER B. J. and WAINWRIGHT T. E., *Phys. Rev. A*, 1 (1970) 18.
[2] LEVESQUE D. and ASHURST W. T., *Phys. Rev. Lett.*, 33 (1974) 277.

[3] ERPENBECK J. J. and WOOD W. W., *Phys. Rev. A*, **26** (1982) 1648.
[4] ERPENBECK J. J. and WOOD W. W., *Phys. Rev. A*, **32** (1985) 412.
[5] ERNST M. H., HAUGE E. H. and VAN LEEUWEN J. M. J., *Phys. Rev. A*, **4** (1971) 2055.
[6] DORFMAN J. R. and COHEN E. G. D., *Phys. Rev. Lett.*, **25** (1970) 1257; *Phys. Rev. A*, **6** (1972) 776; **12** (1975) 292.
[7] FRISCH U., HASSLACHER B. and POMEAU Y., *Phys. Rev. Lett.*, **56** (1986) 1505.
[8] FRISCH U., D'HUMIÈRES D., HASSLACHER B., LALLEMAND P., POMEAU Y. and RIVET J.-P., *Complex Systems*, **1** (1987) 649.
[9] FRENKEL D., in *Proceedings of Workshop on Cellular Automata and Modelling of Complex Physical Systems, Les Houches, France, February 21-28, 1989*, edited by P. MANNEVILLE (Springer, Berlin) 1989.
[10] FRENKEL D. and ERNST M. H., *Phys. Rev. Lett.*, **63** (1989) 2165.
[11] VAN DER HOEF M. A. and FRENKEL D., *Phys. Rev. A*, **41** (1990) 4277.
[12] VAN DER HOEF M. A. and FRENKEL D., *Physica D*, **47** (1991) 191.
[13] VAN DER HOEF M. A. and FRENKEL D., *Phys. Rev. Lett.*, **66** (1991) 1591.
[14] ERNST M. H., *Physica D*, **47** (1991) 198.
[15] D'HUMIÈRES D., LALLEMAND P. and FRISCH U., *Europhys. Lett.*, **2** (1986) 291.
[16] RIVET J.-P., HÉNON M., FRISCH U. and D'HUMIÈRES D., *Europhys. Lett.*, **7** (1988) 231.
[17] NAITOH T., ERNST M. H., VAN DER HOEF M. A. and FRENKEL D., *Phys. Rev. A*, **43** (1991) in press.
[18] BRITO R. and ERNST M. H., to be published.
[19] D'HUMIÈRES D., QIAN Y. H. and LALLEMAND P., in *Proceedings of Workshop on Discrete Kinetic Theory, Lattice Gas Dynamics and Foundation of Hydrodynamics, Torino, Italy, September 20-24, 1988*, edited by R. MONACO (World Scientific) 1989.