Zeitschrift: Helvetica Physica Acta

Band: 65 (1992)

Heft: 2-3

Artikel: Long-time dynamics of two-dimensional fluid binary mixture in cellular automata models

Autor: Perera, A. / Penson, K.A. / Schultze, U.

DOI: https://doi.org/10.5169/seals-116501

Long-Time Dynamics of Two-Dimensional Fluid Binary Mixture in Cellular Automata Models

A. Perera, K. A. Penson, U. Schultze and M. Moreau
Université Pierre et Marie Curie
Laboratoire de Physique Théorique des Liquides
Tour 16, 5eme et. Boîte 121
F-75252 Paris Cedex 05, France.

Abstract. We compute exponents of long-time tails of the velocity auto-correlation functions in binary mixtures in cellular automata models in 2D using numerical simulations. The exponents are found to vary with densities as opposed to universal values for the one component system.

The idea of applying the model system in which both space and time are discrete, to obtain properties of fluids, had proven highly successful. Following the seminal work of Frisch, Hasslacher and Pomeau (FHP) [1] very large number of problems have been treated with such cellular automata (CA) models. For recent references consult an exhaustive review article [2] and Ref. [3]. The problem of long-time tails of the velocity correlation function $\phi(t) =< \vec{v}(0)\vec{v}(t) >$ (VACF) has received increased attention. Recently, with a newly conceived rapid simulation method by van der Hoef and Frenkel [4] , the prediction of mode-coupling theory $\lim_{t\to\infty} \phi(t) \sim t^{-D/2}$ has been for the first time confirmed for a single component CA fluid in 2D and 3D [4].

Here we report simulation results applying the methods of ref.[4] on a CA representation of fluid binary mixture of unequal species, called heavy (H) and light (L) on a 2D triangular lattice.

As usual in CA model the interactions are specified by a set of collision rules : a) the state of H particles is not affected by the presence of L particles. H particles interact between themselves according to FHP-III collision rules [1],[2]; b) if a lattice node is occupied only by L particles, they interact also according to FPH-III rules; c) if a node is occupied by at least one H particle, the L particles are scattered off H particles randomly; d) no two particles can propagate on the same link and the same direction (exclusion principle).

This model is a generalization of the Lorentz gas [5] : the scattering centers for L particles are H particles. The latter can move and display their own dynamics governed by collisions with other H particles. Obviously the dynamics of L particles is our main interest here. When the density of L particles is low and that of H particles quite high the diffusion of the former will be analogous to a random walk. Indeed we find numerically that the VACF decays exponentially.

The most interesting case arises when either the two densities ρ_H and ρ_L of respectively heavy and light particles are either comparable or when $\rho_H \leq \rho_L$. We find in fact that, in the case of our model, the VACF for L particles has a long-time tail with an exponent which depends on ρ_H and ρ_L in a non trivial way.

Fig.1 shows a plot of $\log \phi(t)$ versus $\log t$ for the particular case of $\rho_H = 0.4$ and for $\rho_L = 0.2$ and $\rho_L = 0.4$. We see that in both cases the exponent of the long-time tail is clearly smaller than unity. This is an opposite behaviour of the static Lorentz gas where the exponent was found to be 2 [6]. The full parameter space of ρ_H and ρ_L ($\rho_H + \rho_L \leq 1$) is being currently explored.

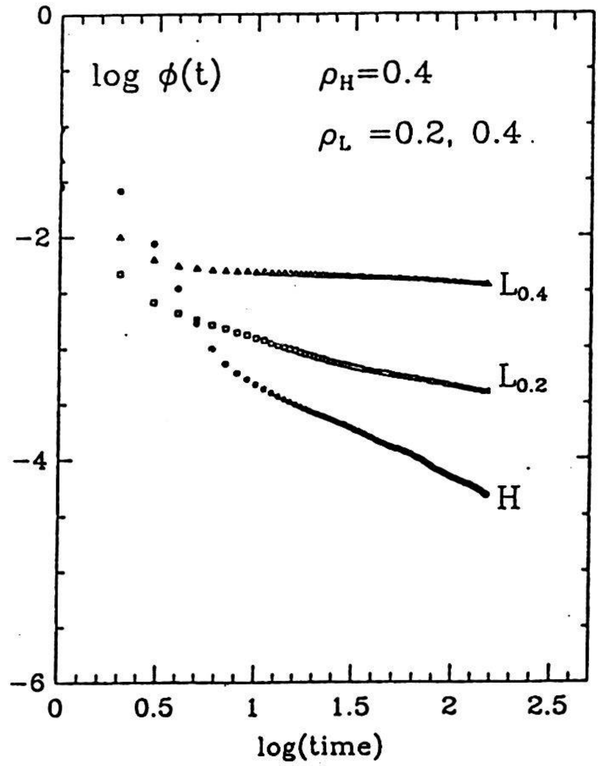

Fig.1 : Log-log plot of the VACF's for densities specified in the inset.

References

1) U. Frisch,B. Hasslacher and Y. Pomeau, Phys. Rev. Lett. 56, 1505 (1986).

2) M. H. Ernst, in "Liquid, Freezing and the Glass Transition.", Les Houches , Session LI, D. Levesque, J. P. Hansen and J. Zinn-Justin, Eds. (North Holland. 1991).

3)"Lattice Gas Methods for Partial differential equations", G. D. Dolan, Ed. (Addison-Wesley ,1990)

4) M. A. van der Hoef and D. Frenkel, Phys. Rev. A 41, 4277 (1990).

5) A. Perera, B. Gaveau, M. Moreau and K. A. Penson, Phys. Lett. A, in press.

6) P.-M. Binder and D. Frenkel, Phys. Rev. A 42, 2463 (1990).