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II. VELOCITY CORRELATION FUNCTIONS

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THE PROPERTIES OF TAGGED LATTICE FLUIDS:
II. VELOCITY CORRELATION FUNCTIONS

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ABSTRACT

We report preliminary measurements of the velocity autocorrelation function for a tagged particle in a lattice gas. These measurements agree with the Boltzmann-level theory. The Green-Kubo integration of these measurements agrees with theoretical predictions for the diffusion coefficient. To within the error bars of the simulations (3x 10^{-3}) we observe no long-time tails.

As the theory of lattice gases develops, several measurements of velocity autocorrelation functions, which are an essential ingredient in the Green-Kubo formulae for transport coefficients[1], have been reported in the literature[2-4].

The standard lattice gas models in the square[2] and triangular [5] lattices, henceforth HPP and FHP respectively, have collision rules which do not conserve particle identity. For this reason, the velocity correlation functions that Colvin et al.[3] and Margolus et al.[4] report for lattice gases correspond to hydrodynamic or site correlations rather than to the one-particle correlation functions needed in the Green-Kubo formulation. Both kinds of correlation usually have algebraic long-time tails, the first through the decay of single hydrodynamic modes, the second through the product of modes. Often the algebraic exponent is the same for both, although the amplitude of the latter is considerably smaller; it has been conjectured[6] that isotropy of the viscosity tensor is a necessary condition for the equality in the exponents of both correlation functions [1]. In this paper we report preliminary measurements of the one-particle velocity correlation function for a lattice gas model which we have modified to conserve the individuality of one particle[7,8]. This model is interesting in that the viscosity tensor is not isotropic [2], so that the long-time tails, if they exist, need not be the same as those reported for the site correlation functions in references 2 and 3.

The model we study here is model III of the previous paper in this volume, id est, the HPP model with one tagged particle which deflects left or right at two-body head-on collisions according to the parity of the time step. This particle is representative of any fluid particle in the system. For this model,

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[1] The logarithmic divergence measured in the viscosity of hexagonal lattice gases and accompanying mode-coupling theory by Kadanoff, McNamara and Zanetti, University of Chicago preprint (1987), are consistent with this statement.

[2] See the article on invariants in lattice gases by D.d'Humières and P.Lallemand in this volume.

the Boltzmann level description of reference 8 appears to be adequate at all densities for the calculation of the self-diffusion coefficient.

We have performed simulations of this model for densities of 0.125, 0.25, 0.50 and 0.75 of the maximum of 4 particles per node. 80000 independent trajectories were run for each density value, in the 256 x 512-node periodic field provided by the RAP lattice gas machine. To account for some of the invariants of the system and guarantee no drift, we forced the momentum along each row and column to be exactly zero. No such provisions were taken towards checkerboard or diagonal invariants such as those described by d'Humières and Lallemand in this volume

Based on the Zwanzig-Ailawadi estimate[9], this number of trajectories is enough for an accuracy of one part in 200 in the velocity autocorrelation function. To this accuracy we could check that it obeys the equation

$$\Phi(t) = [1 - c(1 - c)^2]^t \tag{1}$$

presented in the previous paper in this volume, for about 24 time steps. Table 1 contains the best fits for $[1 - c(1 - c)^2]$ from simulations and the diffusion coefficient value that results from the Green-Kubo integration of this value. The last column has the Boltzmann-level result for the diffusion coefficient, which can also be found in the previous paper. We observe excellent agreement between theory and simulations. The Green-Kubo results also agree very well with the Einstein equation measurements of the diffusion coefficient reported in the preceding paper.

Table 1: Density, best exponential fit of the velocity correlation function, values of the diffusion coefficient from experimental Green-Kubo and theoretical methods.

Density	$[1 - c(1-c)^2]$	D(Green-Kubo)	D(Boltzmann)
1/8	0.9077	5.17 ± 0.3	4.95
1/4	0.8682	3.54 ± 0.2	3.3
1/2	0.8826	4.0 ± 0.2	3.8
3/4	0.9545	10.7 ± 0.6	10.5

Figure 1 is a plot of the logarithm of the measured velocity correlation function vs time for a particle density of 0.6. This density seems to provide the best tradeoff between low enough density for the Boltzmann description to be accurate, and high enough density to have meaningful results for at least a few mean-free paths. We have performed 225000 independent simulations for this density. The exponential decay law is obeyed to within the error bars of 0.003, with no evidence of long-time tails. It will be instructive for the reader to compare this plot with those for the site correlation function for the same model, given in references 2 and 4.

We have presented preliminary measurements of the particle velocity autocorrelation function of a tagged version of the HPP model. We obtain very good agreement with theoretical results. We compare the Green-Kubo integration of these measurements with the Boltzmann-level predictions for the diffusion coefficient and obtain excellent agreement. We observe no long-time tails to the level of accuracy of the simulations, which comes as no surprise since these tails are of the order $10^{-3} - 10^{-4}$.

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Figure 1: Natural logarithm of the particle velocity autocorrelation function vs. time for a tagged-particle HPP gas, density=0.6, 225000 simulations.