Long- and ultimate-time tails in two-dimensional fluids

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In a recent comment [J. A. Leegwater and G. Szamel, Phys. Rev. Lett. **67**, 408 (1991)] we showed that the $(t\sqrt{\ln t}\,)^{-1}$ decay of the velocity-autocorrelation function in a two-dimensional lattice gas should be attained in times accessible in simulations. Here we study in greater detail the properties of solutions to the self-consistent mode-coupling equations on which this result was based. We propose a scenario for the decay of the velocity autocorrelation function of a two-dimensional lattice-gas cellular automaton.

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I. INTRODUCTION

It has been known for more than 20 years that the velocity-autocorrelation function (VACF) of a fluid does not decay exponentially, as was expected on the basis of the Boltzmann equation, but rather algebraically at long times. Mode-mode-coupling theory gives that in d dimensions the decay is proportional to $\phi(t) = \alpha_D[(D+\nu)t]^{-d/2}$, where D is the self-diffusion coefficient, ν the shear viscosity, and α_D a prefactor [1]. As the self-diffusion coefficient is equal to the time integral of the VACF, in two dimensions D diverges and a more refined treatment is needed. The self-consistent (SC) equations, such as those written down below, predict that for long times the VACF is proportional to $t^{-1}(\ln t)^{-1/2}$, as was first established by Wainwright, Alder, and Gass [2] and Kawasaki [3]. Recently, van der Hoef and Frenkel [4] found evidence for a faster-than-t^{-1} decay of the VACF in a two-dimensional (2D) lattice-gas cellular automaton (LGCA). They showed that this decay is compatible with the onset of self-consistent effects in the long-time tails [5]. The model they used was the so-called FHP-III (third version of the Frisch-Hasslacher-Pomeau model); for a detailed description of this model, and LGCA in general, we refer to the literature [6]. Naitoh, Ernst, and Dufty [7] recently derived the self-consistent equations for the FHP-III model, with coefficients, using mode-mode-coupling theory. Naitoh, Ernst, and Dufty, as well as van der Hoef and Frenkel, estimated the time after which self-consistent effects are large, to be of the order of 10^{20} lattice times. Times accessible in simulations are of the order of 10^3 and logarithmic corrections for these times are of the order of 15%.

On the basis of the time estimate mentioned it was assumed that it would be impossible to observe the self-consistent tail in simulations. However, we pointed out the following in a recent comment [8].

(i) The solution to the self-consistent equations produces a VACF that is approximated to within 1% by

$$\phi(t) = \frac{A}{t[\ln(tt_u/t_f^2)]^{1/2}} \tag{1}$$

for an extremely long-time period and lattice fillings $f \geq 0.5$. The relation to the previous estimate is that t_u is very large, at least of the order of 10^{20} mean free times, so the value of the logarithm changes only slightly for times accessible in simulations. In Eq. (1) t_f is the mean free time, which is of the order of 1 in lattice units.

(ii) The coefficient A appearing in (1) is not equal to the value ultimately obtained. The times for which (1) is still accurate is extremely long though, at least of the order of 10^{100}. We could not establish an accurate value for the time at which the ultimate-time tail expression is the one to use, as the computer on which the calculations were done cannot treat numbers larger than 10^{300}.

In this article we present a more detailed analysis. The results mentioned were established assuming that the self-consistent mode-mode-coupling theory is correct, and that the coefficients as calculated by Naitoh, Ernst, and Dufty are accurate. A major part of the results of this article will also be valid for other 2D fluids for which similar self-consistent equations hold; we illustrate this for a hard-disk fluid.

II. HALF-FILLED LATTICE

Consider the mode-mode-coupling theory prediction for the long-time tail of the VACF ϕ which is assumed to hold after some time t_0:

$$\phi(t) = \frac{\alpha_D}{(\bar{D}+\bar{\nu})t}\ , \tag{2}$$

$$D(t) = \int_0^t dt_1 \phi(t_1)\ , \tag{3}$$

$$\bar{D}(t) = \frac{1}{t}\int_0^t dt_1 D(t_1)\ , \tag{4}$$

where D is the self-diffusion coefficient, and ν the kinematic shear viscosity. In this section we study the half-filled lattice, for which the shear viscosity is predicted to be finite by Naitoh, Ernst, and Dufty. In this case the set of equations (2)–(4) is closed. The expressions for the "bare," or short-time transport coefficients that are used here are taken from the literature [9,10]. The time-scale estimate mentioned is arrived at as follows. For SC effects to be large the contribution from the tail in Eq. (3) must be comparable to that of the short-time regime. So to get a rough estimate of the self-consistent time scale t_s, we take the time at which

$$\int_{t_0}^{t_s} dt_1 \frac{\alpha_D}{(D_0+\nu_0)t_1} = \tfrac{1}{2}D_0 \tag{5}$$

[the factor $\frac{1}{2}$ is motivated by Eq. (8) below] or

$$t_s = \exp\left[\frac{D_0(D_0+\nu_0)}{2\alpha_D}\right] t_0 \simeq 10^{26} t_0 , \tag{6}$$

where the numerical value applies at lattice filling $f=0.5$. The time t_0 is the time scale after which Eq. (2) is expected to hold, and is somewhere in between 1 and 100 mean free times (see Sec. IV). The order of magnitude of the time t_u in Eq. (1) is similar to that of t_s.

A solution of the self-consistent equations can be obtained in closed form as follows. Define a new variable $a=t(\overline{D}+\nu)$. The SC equations transfer into

$$\frac{d^2}{dt^2}a(t) = \frac{\alpha_D}{a} \tag{7}$$

of which the solution is

$$\frac{d}{dt}a = (2\alpha_D \ln a + b)^{1/2} , \tag{8}$$

with b an integration constant. Equation (8) can be regarded as an explicit differential equation for t in terms of a. The resulting integral can be performed yielding

$$t = t_1 + \frac{\sqrt{2\alpha_D}}{\phi_0}\Phi(\sqrt{\ln\phi_0/\phi}) , \tag{9}$$

where t_1 and ϕ_0 are determined by the initial values, and

$$\Phi(z) = \int_0^z e^{t^2} dt = -i\frac{\sqrt{\pi}}{2}\,\mathrm{erf}(iz) . \tag{10}$$

More insight into the solution can be obtained by rewriting the SC equations in terms of new variables

$$x = [t\phi(t)]^{-2} \tag{11}$$

and

$$y = \alpha_D x \left[\frac{t(D+\nu)\phi}{\alpha_D} - 1\right] . \tag{12}$$

In logarithmic time $\tau = \ln t$ we find

$$\frac{dx}{d\tau} = \frac{2}{\alpha_D} y , \tag{13}$$

$$\frac{dy}{d\tau} = 1 - y + \frac{y^2}{\alpha_D x} . \tag{14}$$

Now the initial values for x and y are such that the last term in (14) is small (0.01 at lattice filling $f=0.7$), hence y tends to unity exponentially on a logarithmic time scale. This peculiarity of the self-consistent equations causes the long-time regime to be reached much earlier than the previous estimate. The resulting VACF at half-filled lattice is given as the solid line in Fig. 1. The function x is defined such that on this plot a straight line corresponds to a $(t\sqrt{\ln t})^{-1}$ tail. The dotted line is a straight line with a coefficient that corresponds to the ultimate-time tail. Only for relatively short times there are notable deviations; after 10^5 lattice times we are in the ultimate-time regime.

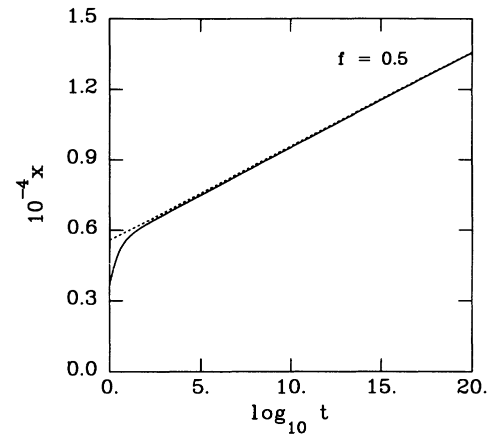

FIG. 1. The function $x=(t\phi)^{-2}$ calculated using the self-consistent equations at half-filled lattice. Solid line, numerical solution; dotted line, linear interpolation with the long-time coefficient. Already for a surprisingly short time, the long-time behavior is reached.

III. COUPLED SELF-CONSISTENT EQUATIONS

Only at half-filled lattice the shear viscosity is finite, and for other densities we need to solve the full set of self-consistent equations, as they are given in [7]. The numerical solution has been presented in Ref. [8]; it turned out that the $(t\sqrt{\ln t})^{-1}$ tail is accurate much longer than could naively be expected. However, its magnitude is different from the value ultimately obtained, as calculated by Naitoh, Ernst, and Dufty. We found that the transition to the ultimate-time tail is extremely slow. Here we study a simplified model in order to try to understand this finding. Assume that for the shear viscosity the SC equations of the form (2)–(4) hold with a coefficient α_ν, so that after a transient we have

$$\overline{\nu}(t) = (\nu_0^2 + 2\alpha_\nu \ln t)^{1/2} , \tag{15}$$

where ν_0 is the short-time, or Boltzmann, viscosity, and α_ν the coefficient to the long-time tail. Regarding Eq. (2) we approximate $\overline{\nu}$ in this model, rather than the time-dependent viscosity ν. Then Eq. (13) is not changed, and (14) has to be replaced by

$$\frac{dy}{d\tau} = 1 - y + \frac{y^2}{\alpha_D x} + \frac{\alpha_\nu\sqrt{x}}{\overline{\nu}} . \tag{16}$$

Some analytical asymptotic results can still be established for these equations. Notice that for long times y will tend to a constant and the term proportional to y^2 becomes negligible. Up to small corrections y is given by the value obtained by setting $dy/dt=0$, which is a quasistationary approximation for y. So take

$$\overline{y} = 1 + \alpha_\nu\left[\frac{x}{\nu_0^2 + 2\alpha_\nu \tau}\right]^{1/2} , \tag{17}$$

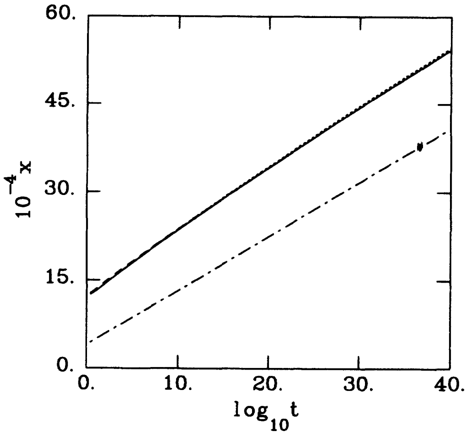

FIG. 2. The function $x=(t\phi)^{-2}$ resulting from the model Eq. (15). In this figure the following values were used (in lattice units): $v_0=0.1$, $D_0=0.25$, $\alpha_D=10^{-3}$, and $\alpha_v=5\times10^{-4}$. These are realistic values which are roughly appropriate for lattice filling $f=0.7$. The numerical solution to the SC equations (2) and (16) is the solid line, the quasistationary approximation Eq. (17) yields the dashed line, which is only distinguishable from the solid line for small $\ln t$. Also plotted are the linear term of (20) (dash-dotted) and the full expression where C was fitted such that x is reproduced at $\tau=8$ (dotted). Notice that the solid, dashed, and dotted lines are barely distinguishable, and that the second term of (20) is quite large, at least on these time scales. For the parameters used the nonuniversal exponent is 0.25.

which in Fig. 2 is shown to yield a very accurate approximation to the solution of the full equation (15). Redefine τ so that the v_0^2 cancels. The SC equations in the quasistationary approximation in terms of a new time $s=2\tau/\alpha_D+v_0^2/\alpha_D\alpha_v$ are transformed into

$$\frac{dx}{ds}=1+\lambda\sqrt{x/s}\ , \tag{18}$$

with $\lambda=\sqrt{\alpha_v/\alpha_D}$. The solution of (18) follows, after some algebra, as

$$\left[\frac{s}{s_0}\right]^{-(1+\lambda^2/4)^{1/2}}=\left|\sqrt{x/s}-\lambda_1\right|^{\lambda_1}\left[\sqrt{x/s}-\lambda_2\right]^{-\lambda_2}, \tag{19}$$

where $\lambda_{1,2}=\lambda/2\pm(1+\lambda^2/4)^{1/2}$, and s_0 is an integration constant. For $s\to\infty$ the left-hand side will tend to zero. As λ_2 is negative, and the square root is positive, for long times $\sqrt{x/s}$ will tend to λ_1. It can be established that for long times

$$x=\frac{2}{\alpha_D}\lambda_1^2\left[\tau+\frac{v_0^2}{2\alpha_v}\right]+C\left[\tau+\frac{v_0^2}{2\alpha_v}\right]^{\lambda/2[(1+\lambda^2/4)^{1/2}-\lambda/2]}+\cdots\ . \tag{20}$$

Notice that the second term has a nonuniversal exponent. A typical plot is presented in Fig. 2. The second term in Eq. (20) is large on physical time scales, but decays extremely slowly, partly explaining the slow transition to the ultimate-time tail. We believe that this is the generic behavior for coupled self-consistent equations.

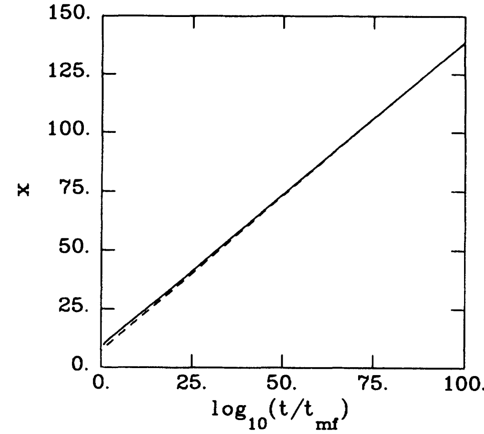

FIG. 3. The function x as a function of time divided by the mean free time $t_{\rm mf}$, obtained by numerically solving the full set of self-consistent equations for a hard-disk fluid at density $n\sigma^2=0.1$ using Boltzmann transport coefficients. Solid line, solution to self-consistent equations; dashed line, a straight line indicating the asymptotic solution.

IV. FINAL REMARKS

The full set of self-consistent equations as they apply to a lattice gas are a complicated set of five coupled equations. The numerical solution is this set of equations can be found in Ref. [8]. To show that the phenomena discussed there are not peculiarities of lattice gases we have numerically calculated the long-time tail for a hard-disk fluid in the low-density limit, using the self-consistent modification of the expressions given in Ref. [11]. The result is shown in Fig. 3. For hard disks the "short" long-time tail is already the asymptotic tail, reminiscent of the half-filled lattice.

Based mainly on the work described in [8] and Fig. 2, we arrive at the following scenario for the VACF of a 2D LGCA. There are four time scales: (i) The short-time regime, where the Boltzmann theory is accurate. For a lattice gas at reasonably high lattice filling this is of the order of two lattice times. (ii) A transition regime, for which all kinds of effects have to be included, such as sound modes and extended mode-mode coupling effects. Recently this time regime was studied by Naitoh *et al.* [12]. The results of van der Hoef and Frenkel [4] as well as the present calculations suggest that also the onset of self-consistent effects has to be taken into account. (iii) A time regime where Eq. (1) is accurate. This time regime can be estimated to range from 100 to at least 10^{100} lattice times. (iv) An ultimate-time regime, for which Eq. (1) should hold with the coefficients as calculated by Naitoh *et al.* In this paper we could not resolve the question of when or how this regime is attained.

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