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Stochastic rotation dynamics: A Galilean-invariant mesoscopic model for fluid flow

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A recently introduced stochastic model for fluid dynamics with continuous velocities and efficient multiparticle collisions is investigated, and it is shown how full Galilean-invariance can be achieved for arbitrary Mach numbers. Analytic expressions for the viscosity and diffusion constant are also derived and compared with simulation results. Long-time tails in the velocity and stress autocorrelation functions are measured.

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Hydrodynamic simulations of complex liquids such as amphiphilic mixtures and polymeric liquids remain a major challenge. For these fluids, mesoscopic simulation methods are often more efficient and stable than conventional computational fluid dynamics algorithms; in addition, they have shown great promise for simulating flow in complicated geometries. For these reasons, there has been a considerable effort to develop lattice gas automata (LGA) [1], lattice-Boltzmann (LB) methods [2], and particle-based mesoscopic simulation techniques such as dissipative particle dynamics (DPD) [3].

In the LGA method, the fluid is modeled as a collection of particles which move along the links of a regular lattice and interact according to well-defined collision rules. If these collision rules preserve mass and momentum conservation, the correct hydrodynamic behavior can be obtained at macroscopic length scales. In the LB method, the time development of particle distribution functions with a set of fixed lattice velocities on a regular lattice is described by a discretized LB equation. Both of these lattice methods are very efficient due to the simplified collision dynamics and strong reduction of velocity space. However, this reduction is also their major drawback: they are not Galilean-invariant, a problem which restricts their use to conditions in which the flow velocity is small compared to the maximum lattice velocity. In addition, the LB approach is subject to a number of numerical instabilities. While off-lattice methods such as DPD do not suffer from these drawbacks, they are often complex and difficult to analyze analytically.

Recently, a promising particle-based method for simulating fluid flow (which we will call stochastic rotation dynamics) was introduced by Malevanets and Kapral [4]. The fluid is modeled by particles whose positions and velocities are continuous variables. The system is coarse-grained into the cells of a regular lattice and there is no restriction on the number of particles in a cell. The evolution of the system consists of two steps: streaming and collision. In the streaming step, the coordinate of each particle is incremented by its displacement during the time step. Collisions are modeled by a stochastic rotation of the relative velocities of every particle in each cell. The dynamics is explicitly constructed to conserve mass, momentum, and energy, and the collision process is the simplest consistent with these conservation laws. It has been shown that there is an *H*-theorem for the dynamics and that this procedure yields the correct hydrodynamic equations for an ideal gas [4]. However, many fundamental questions regarding this approach still need to be answered before it can be applied with confidence. In this Rapid Communication we address these questions and present the results of a detailed analytic and numerical study of this model. In particular, the validity of the assumption of molecular chaos made in Ref. [4] is critically analyzed, and it is shown that the original algorithm is not Galilean-invariant at low temperatures. We then show how the algorithm needs to be modified in order to guarantee Galilean-invariance at *arbitrary* Mach and Schmidt numbers and determine the dependence of the transport coefficients on the mean free path and rotation angle. New analytical expressions for the transport coefficients at small and large mean free path are also derived and compared with simulations results.

Consider a set of N point-particles with (continuous) coordinates $\mathbf{r}_i(t)$ and velocities $\mathbf{v}_i(t)$ in two dimensions. In the streaming step all particles are propagated simultaneously a distance $\mathbf{v}_i\delta$, where δ is the value of the discretized time step. For the collision step, particles are sorted into cells, and they interact only with members of their own cell. The simplest cell construction is a square grid with mesh size a. However, as will be shown, a shortcoming of imposing this lattice structure is that it can lead to a breakdown of Galilean-invariance, as well as other anomalies. The macroscopic velocity $\mathbf{u}(\boldsymbol{\xi},t)$ is defined as the mean velocity of the particles in the cell with coordinate $\boldsymbol{\xi}$. The local temperature, T, is given by the mean square deviation of the velocities from the macroscopic velocity, $\mathbf{u}$.

The collision step consists of a random rotation of the relative velocities, $\mathbf{v}_i-\mathbf{u}$, of each particle in a cell by an angle $\pm\alpha$. All particles in the same box are subject to the same rotation, but the rotation angles of different cells are statistically independant. The local momentum and kinetic energy is invariant under this operation. The dynamics is summarized by

$$\mathbf{r}_i(t+\delta)=\mathbf{r}_i(t)+\delta\,\mathbf{v}_i(t), \tag{1}$$

$$\mathbf{v}_i(t+\delta)=\mathbf{u}+\boldsymbol{\omega}\cdot\{\mathbf{v}_i(t)-\mathbf{u}\}, \tag{2}$$

where $\boldsymbol{\omega}$ denotes a stochastic rotation matrix which rotates by an angle of either $+\alpha$ or $-\alpha$ with probability 1/2.

A series of simulations were performed on systems with periodic boundary conditions and L^2 cells with L ranging from 16 to 64. The average number of particles per cell, M,

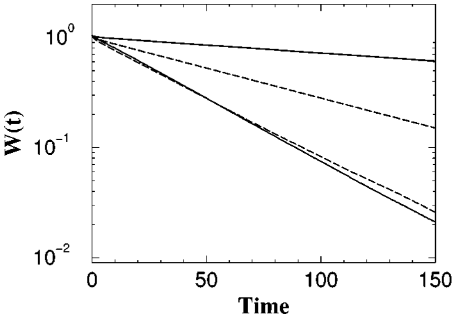

FIG. 1. Vorticity correlations W vs time for two different wave vectors **k** at small mean free path, $\Lambda = 0.11$, with (dashed lines) and without (solid lines) the random shift of the grid. The upper solid and dashed lines are results for $\mathbf{k} = 2\pi(0,1)/L$. The lower solid and dashed lines correspond to $\mathbf{k} = 2\pi(1,1)/L$. Parameters: $T = 0.01275$, $\alpha = 90°$, $M = 35$, and $L = 16$.

was between 5 and 70. The simulations were started with a random distribution of particles with random initial velocities with components in the interval $\pm v_{max}$. The velocity distribution quickly relaxes to a Maxwell-Boltzmann distribution with an essentially temperature independent relaxation time $\tau \propto M$. τ was found to depend strongly on the value of the rotation angle α, and to diverge approximately as $\tau \sim \alpha^{-2}$ for $\alpha \rightarrow 0$; in this limit, there are no collisions and thermal equilibrium can never be achieved.

In order to determine the kinematic shear viscosity, ν, the temporal correlations of the vorticity, $w_k = k_x \tilde{u}_y - k_y \tilde{u}_x$, were measured, where $\tilde{u}_x$ is the Fourier transform of the x component of the macroscopic velocity. According to fluctuating hydrodynamics, vorticity correlations decay as $\langle w_k(t) w_{-k}(0) \rangle \sim \exp[-\nu(k) k^2 t]$. We found that the value of ν determined in this way is at least a factor of 2 larger than that given by Eq. (47) of Ref. [4] for $\alpha = 90°$. In addition, we found an anomaly in $\nu(k)$ if one component of the wave vector is zero. It can be seen in Fig. 1 (solid lines) that the viscosity at wave vector $\mathbf{k} = 2\pi(1,0)/L$ is approximately four times smaller than for $2\pi(1,1)/L$. Imposing a homogenous flow parallel to the wave vector $\mathbf{k}_0 = (k_x, 0)$ leads to a similar drastic change in the value of $\nu(\mathbf{k}_0)$. Another manifestation of this breakdown of Galilean-invariance was observed when measuring the diffusion constants D_x, D_y of particles in the x and y directions in the presence of a homogenous flow field. It was found that D_x/D_y is not always equal to 1.

These artifacts led us to a critical review of the basic assumptions in the analysis in [4], in particular that of *molecular chaos*. Molecular chaos means that particles involved in a collision have no memory of earlier encounters when colliding. This is clearly not the case if the particles travel a distance between collisions which is small compared to the cell size a. In this case, essentially the same particles ''collide'' repeatedly before other particles enter the cell or some of the participating particles leave the cell. Introducing the mean free path, $\lambda = \delta \sqrt{T}$ [5], which is the average distance particles stream between rotations, the assumption of molecular chaos should be valid when $\lambda \gg a$, because most collisions then involve particles which have just arrived from different cells. After a collision, particles immediately leave to other cells, and decorrelate quickly. This behavior is confirmed by our simulations. For example, the ratio of the diffusion constants $R = D_x/D_y$ was measured in a homogeneous flow field as a function of $\Lambda = \lambda/a$. While there are significant deviations from $R = 1$ for small Λ, for $\Lambda > 1/2$, R deviates from one by less than 0.3%.

For small Λ, large numbers of particles in a given cell remain correlated over several time steps. These correlations are changed by the presence of flow, and Galilean-invariance is broken. One way of removing this dependence on the macroscopic velocity is to perform a random shift of the grid before performing the stochastic rotation. If the magnitude of the random components of the shift are on the order of the cell size a, the collision environment of each particle no longer depends on the macroscopic velocity, and it can be shown [6] that there is an exact restoration of Galilean-invariance. This makes it possible to perform simulations at arbitrary Mach number even at low temperature.

In our implementation of this procedure all particles are shifted by the *same* random vector with components in the interval $[-a/2, a/2]$ before the collision step. Particles are then shifted back by the same amount after the collision. This shifting procedure, in conjunction with the stochastic collision, leads to an additional contribution to the viscosity which removes the anomalies in its k dependance. Figure 1 (dashed lines) shows the exponential decay of the vorticity correlations for different wave numbers if the shifting procedure is applied. In contrast to the results obtained without the shift, the short time viscosity is now essentially independant of the wave vector **k**.

In the streaming step, momentum is transfered directly from one cell to another when particles cross cell boundaries. This leads to a kinetic contribution to the viscosity, ν_{kin}, calculated previously [4]. However, as mentioned above, there is also a rotational contribution, ν_{rot}. The total kinematic viscosity therefore consists of the sum of three contributions, $\nu = \nu_{kin} + \nu_{rot} + \nu_{mix}$, where ν_{mix} is a cross term resulting from both streaming and rotation. These additional contributions are zero in the original method, because the rotations do not transfer momentum between different cells. When the shifting procedure is applied, the rotational contribution is nonzero; for $\Lambda \ll 1$, ν_{rot} is the dominant contribution to the viscosity.

In this limit, an approximate expression for $\nu \sim \nu_{rot}$ can be obtained from elementary kinetic theory: Consider M particles in a single cell which is divided into two subcells by a line parallel to the x direction. In each of the subcells, macroscopic velocities $\mathbf{u}_1$ and $\mathbf{u}_2$ can be defined as the average velocity of the subcell particles. In the rotation step, momentum is transfered between the two subcells. This momentum transfer can be easily calculated using Eq. (2). It depends on the rotation angle and the velocity difference $\mathbf{u}_1 - \mathbf{u}_2$. Using the definition of the shear viscosity as the proportionality constant between the momentum transfer and the velocity gradient and averaging over the position of the dividing line, one finds

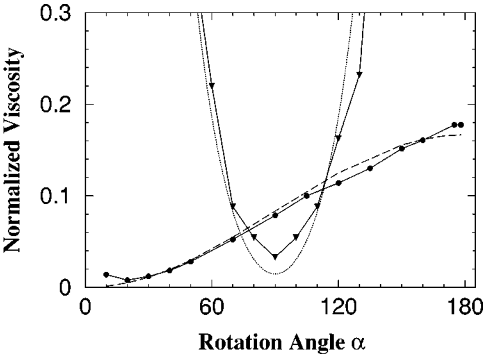

FIG. 2. The normalized kinematic viscosity, ν, measured at short times as a function of the rotation angle α. The bullets show $\nu\delta/a^2$ at small mean free path, $\Lambda=0.028$. The dashed line is expression (3). The filled triangles are $\nu/(\delta T)$ at large mean free path, $\Lambda=4$. For comparison, the dotted line shows Eq. (7). $L=32$ and $M=35$.

$$\nu_{rot}=\frac{a^2}{12\,\delta}[1-\cos(\alpha)]. \qquad (3)$$

Simulation results for the viscosity for $\Lambda=0.028$ are in good agreement with Eq. (3) for rotation angles that are neither too small nor too large, as shown in Fig. 2 (dashed line and •). The angular dependence is qualitatively different at large mean free path, Fig. 2 (dotted line and ▼). The claim in Ref. [4] that the viscosity has a minimum at $\alpha=90°$ is only true for large Λ. For smaller Λ the minimum is shifted to smaller angles. Equation (3) cannot correctly describe the total viscosity at very small and very large angles because the kinetic part of the viscosity becomes large there even if Λ is small.

A Green-Kubo relation can also be used to determine the viscosity. For discretized time, the long wavelength limit of the viscosity can be expressed as [7]

$$\nu(t)=\frac{\delta}{NT}\left(\frac{\langle P_{xy}^2(0)\rangle}{2}+\sum_{l=1}^{n}\langle P_{xy}(l\,\delta)P_{xy}(0)\rangle\right), \qquad (4)$$

where $t=n\delta$ and $P_{xy}(t)$ is the transverse part of the microscopic stress tensor at time t. P_{xy} is defined as the zero wave vector limit of $\partial_t J_{xy}(k_x,t)/(ik_x)$, where J_{xy} is the transverse momentum current [7]. Using Eqs. (1) and (2), and including the random shift of the grid, one finds $P_{xy}=P_{xy}^{kin}+P_{xy}^{rot}$, with

$$P_{xy}^{kin}(t)=\frac{1}{\delta}\sum_{j=1}^{N} v_{j,y}(t)\Delta\xi_{j,x}, \qquad (5)$$

$$P_{xy}^{rot}(t)=\frac{1}{\delta}\sum_{j=1}^{N} \Delta\xi_{j,x}^{S}\Delta v_{j,y}, \qquad (6)$$

with $\Delta\xi_{j,x}=\xi_{j,x}(t+\delta)-\xi_{j,x}(t)$, $\Delta^S\xi_{j,x}=\xi_{j,x}(t+\delta)-\xi_{j,x}^S(t+\delta)$, and $\Delta v_{j,y}=v_{j,y}(t+\delta)-v_{j,y}(t)$. $\boldsymbol{\xi}_j(t)=(\xi_{j,x},\xi_{j,y})$ denotes the coordinates of the cell which contains particle j at time t. $\boldsymbol{\xi}_j^S$ are the temporary cell coordinates in the new randomly shifted reference system. Without the shift procedure, $P_{xy}^{rot}=0$, and rotations do not contribute to the viscosity at zero wave vector. In this case the expression for ν agrees with the one derived by more complicated means in [4]. A series of simulations both with and without the shifting procedure were performed to measure P_{xy} and to calculate the viscosity using Eq. (4). We found that the cross term in the viscosity, ν_{mix}, which measures the correlations between P_{xy}^{rot} and P_{xy}^{kin} is always negative. For large mean free path, $\Lambda\gg 1$, ν_{mix} cancels the rotational contribution to the viscosity, ν_{rot}, and at small Λ, it cancels the kinetic part, ν_{kin}. Viscosities measured at short times using the Green-Kubo expression (4) agree to within 3% with the values determined from measurements of the vorticity correlations.

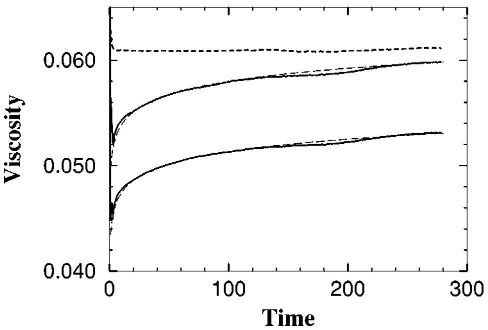

FIG. 3. Various contributions to the viscosity vs time. The kinetic part, ν_{kin}, is represented by the lower solid line, and the total viscosity, ν, by the upper solid line. Both show the same logarithmic behavior. The function $a+b\ln(t)$ is shown for comparison (dashed lines). The deviation at time $t\approx 200$ is due to the recurrence of sound waves because of the small 64×64 system size. The rotational part, ν_{rot}, shown by the top dashed line, is essentially constant at long times. $\alpha=60°$, $\Lambda=0.2$, and $M=5$.

At large times there is a renormalization of the viscosity due to long-time tails in stress correlations [8], and in two dimensions, the viscosity is predicted to diverge logarithmically with time. We were able to directly measure this logarithmic behavior using Eq. (4) (see Fig. 3). We found that only the kinetic part of the stress tensor contributed to the $1/t$ tail in the stress correlation function; no tails could be detected in either the rotational or the mixed contributions. The results are in good agreement with the predictions of mode-coupling theory [8]. The amplitude of the long time tail of the velocity autocorrelation function was measured and also found to agree with theory. A more detailed discussion of these results will be presented elsewhere [6].

Consider now the limit of large mean free path, where the rotational contribution is negligible, i.e., $\nu\approx\nu_{kin}$. In this limit, $\Delta\boldsymbol{\xi}_i/\delta$ in Eq. (5) can be approximated by the particle velocity $\mathbf{v}_i$, and the standard expression for the kinetic stress tensor, $P_{xy}=\Sigma_j v_{j,x}v_{j,y}$, is recovered. Equation (4) can now be evaluated analytically by iterating Eq. (2). If fluctuations in the number of particles in a cell are ignored, molecular chaos is assumed, and it is assumed that any two particles are in the same cell at most once, one finds

$$\nu_{kin}=\frac{T\,\delta}{2}\times\left(\frac{1}{M-1}+\frac{\sin^2(2\alpha)[1+\tan^2(\alpha/2)/M]}{4[1-\cos(\alpha)/M-\cos^2(\alpha)(1-1/M)]^2}\right). \qquad (7)$$

The result for $\alpha=90°$ agrees with Eq. (47) of [4] up to terms of order e^{-M}, which arise from fluctuations in the number of particles in a cell. As mentioned above, our simulation data for $\Lambda=4$ do not agree with this result. The reason for that is that there are temporal correlations extending over more than one time step even at large Λ. In particular, the approximation $P_{xy}\approx\Sigma_j v_{j,x}v_{j,y}$ used in the calculation of $\langle P_{xy}(l\,\delta)P_{xy}(0)\rangle$ is not accurate for small l.

Note that the limit $\alpha=90°$, and $M\rightarrow\infty$, which appears to be a good way to achieve high Reynolds numbers, is pathological; in this case, kinetic stress correlations oscillate in sign and do not decay to zero.

Finally, the diffusion constant D can be calculated using the analogy to a random walk with step size λ. One finds that

$$D=T\delta\left(\frac{1}{2}+\frac{b}{1-b}\right), \tag{8}$$

with $b=1/M+(1-1/M)\cos(\alpha)$. Measured values of D were found to be in good agreement with Eq. (8) for α not too large. It follows that the Schmidt-number, $Sc=\nu/D$, is smaller than or on the order of one for large mean free path. For $\Lambda\ll1$, however, very large Schmidt-numbers can be obtained since $Sc\sim\Lambda^{-2}$. Sc can be increased further by going to larger rotation angles where D becomes very small.

In this paper it was shown how a random shift of the cell coordinates during the collision step can be used to ensure full Galilean-invariance of the stochastic rotation dynamics model introduced in [4], even at low temperatures. Different analytical expressions for the viscosity were derived which were shown to be in good agreement with simulation results, and the long-time tails of the velocity and stress autocorrelation functions were measured and compared to mode-coupling theory. A simple analytic expression for the diffusion constant was also derived, and it was shown that by varying the mean free path and the rotation angle it is possible to simulate fluids with a wide range of Schmidt numbers.

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

[2] G.R. McNamara and G. Zanetti, Phys. Rev. Lett. **61**, 2332 (1988).

[3] I. Pagonabarraga, M.H.J. Hagen, and D. Frenkel, Europhys. Lett. **42**, 377 (1998).

[4] A. Malevanets and R. Kapral, J. Chem. Phys. **110**, 8605 (1999); **112**, 7269 (2000).

[5] Here and in the following we have set Boltzmann's constant and the particle mass equal to 1.

[6] T. Ihle and D. M. Kroll (unpublished).

[7] D.J. Evans and G.P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic Press, London, 1990).

[8] M.H. Ernst, E.H. Hauge, and J.M.J. van Leeuwen, Phys. Rev. Lett. **25**, 1254 (1970).