Long Wavelength Instability for Uniform Shear Flow

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Uniform shear flow is a prototype nonequilibrium state admitting detailed study at both the macroscopic and microscopic levels via theory and computer simulation. It is shown that the hydrodynamic equations for this state have a long wavelength instability. This result is obtained first from the Navier-Stokes equations and shown to apply at both low and high densities. Next, higher order rheological effects are included using a model kinetic theory. The results are compared favorably to those from Monte Carlo simulation.

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In spite of extensive formal theory for nonequilibrium statistical mechanics, definitive tests and controlled illustrations outside the domain of linear response are rare. One such rare case is the macroscopic state of *uniform* shear flow. Like planar Couette flow the x component of the average flow velocity varies linearly in the y direction. However, the flow is generated by periodic boundary conditions in the local Lagrangian frame [1–3] leading to a uniform temperature and pressure, with a monotonic increase of the temperature. This is in contrast to planar Couette flow, driven by local boundary conditions, for which the temperature is nonuniform but stationary [4]. The advantage of uniform shear flow is that the boundary conditions allow application of computer simulation methods with periodic imaging to emulate bulk effects for small systems, just as in the simulation of equilibrium states. In addition, there are many theoretical advantages such as the absence of a hydrodynamic boundary layer. The problems associated with increasing temperature can be controlled by the addition of a thermostat so that a steady state with the desired flow field results. During the past fifteen years uniform shear flow has been the focus of attention in most studies of classical nonequilibrium statistical mechanics by a wide range of theoretical and simulation methods [5,6]. It is one of the few means by which rheology and transport far from equilibrium can be studied at the fundamental level. More recently, simulations of uniform shear flow have provided the test for new concepts of nonequilibrium variational principles [7] and for the relationship between transport and chaotic Hamiltonian flows [8].

Although it has been known for more than ten years that uniform shear flow undergoes a transition to an ordered state at large shear rates [9], its stability at smaller shear rates has not been questioned. Our objective here is to report an instability of uniform shear flow at any shear rate for a sufficiently long wavelength perturbation. More precisely, solutions to the hydrodynamic equations linearized about the macroscopic state of uniform shear flow show exponential growth in time for wave numbers smaller than a critical wave number $k_{\rm cr}(a) > 0$ for $a > 0$. For the case of zero shear rate these linear equations define the hydrodynamic modes which describe how small perturbations of the velocity, temperature, and density fields decay back to equilibrium. These are the two sound modes, a heat mode, and two shear modes. In a similar way the hydrodynamic modes describing response to perturbations of any reference stationary state can be identified. If all such modes decay in time, the reference stationary state is referred to as linearly stable; conversely, if one or more modes leads to an increasing amplitude in time the reference state is linearly unstable.

The hydrodynamic equations are approximations to the more general local conservation laws for the mass, energy, and momentum densities,

$$D_t n + n\nabla \cdot \mathbf{U} = 0, \quad (1)$$

$$D_t e + (e + p)\nabla \cdot \mathbf{U} + \nabla \cdot \mathbf{S} + P_{ij}\partial_i U_j = w, \quad (2)$$

$$D_t U_i + \rho^{-1}\partial_i p + \rho^{-1}\partial_j P_{ij} = 0, \quad (3)$$

where $D_t \equiv \partial_t + \mathbf{U} \cdot \nabla$ is the material derivative. The momentum density is related to the flow field $\mathbf{U}$ by $\mathbf{g} = \rho\mathbf{U}$, $\rho = mn$ is the mass density (m is the mass and n is the number density), and e is the internal energy density. The pressure p is not an independent variable but is *defined* to have the same functional relationship to n and e as in equilibrium. The inhomogeneous term on the right-hand side of the energy equation is due to an external nonconservative force representing the thermostat. There are several thermostats that have been used in simulations and theory. Here the thermostat is fixed by a force on

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each particle proportional to the velocity relative to the local flow field. Consequently, its average value is zero, and the effect of this force occurs only in the energy equation. The proportionality constant is determined by requiring stationarity for the uniform shear flow state. The resulting term w in Eq. (2) is the same as that obtained using the thermostat for simulations. Finally, the irreversible heat and momentum fluxes are denoted by $\mathbf{S}$ and P_{ij}, respectively. These equations are exact but incomplete until the irreversible fluxes are specified in terms of the hydrodynamic fields. Nevertheless, it is possible to define the state of uniform shear flow without their detailed form. Steady-state uniform shear flow is defined by constant (in both space and time) energy and mass densities, $\{e_0, \rho_0\}$, and a flow velocity whose only nonvanishing component is $U_{0x} = ay$. The constant a is the shear rate and provides the single control parameter measuring the deviation from equilibrium. The boundary conditions are simple periodic conditions in the local Lagrangian coordinate frame, $\mathbf{r}' = \mathbf{r} - \mathbf{U}_0(\mathbf{r})t$. Substitution of these assumptions for e, ρ, and $\mathbf{U}$ into the above conservation laws shows they are all satisfied if $\mathbf{S}$ and P_{ij} are also uniform and the parameter of the thermostat in the energy equation is chosen such that $w_0 = aP_{0xy}$.

Consider small deviations of the hydrodynamic variables from the uniform shear flow state. To be explicit it is necessary to specify the heat and momentum fluxes. We first consider the case for which all spatial gradients are small, including the shear rate a. Then the heat flux is given by Fourier's law, and the momentum flux is given by Newton's viscosity law,

$$\mathbf{S} = -\lambda \boldsymbol{\nabla} T\,, \tag{4}$$

$$P_{ij} = -\eta(\partial_i U_j + \partial_j U_i - \tfrac{2}{3}\boldsymbol{\nabla}\cdot\mathbf{U}\delta_{ij}) - \kappa \boldsymbol{\nabla}\cdot\mathbf{U}\delta_{ij}\,, \tag{5}$$

where λ, η, and κ are the thermal conductivity, shear viscosity, and bulk viscosity, respectively. These are the leading terms in a "uniformity" expansion ordered according to spatial gradients of the hydrodynamic fields [10]. It is convenient to choose density and temperature as independent thermodynamic parameters and to denote the deviations in the hydrodynamic parameters from their values for uniform shear flow by $y_\alpha \equiv \{\delta n, \delta T, \delta U_i\}$. Also, we consider a fluid of hard spheres to specify the equations of state, $e = e(n,T)$ and $p = p(n,T)$. These are determined from the Percus-Yevick equation [11] which is known to be accurate over the entire fluid phase. Combining Eqs. (1)–(5) and retaining terms only up through linear order in y_α identifies the hydrodynamic equations for small perturbations about uniform shear flow. The boundary conditions are made explicit by looking for solutions of the form

$$y_\alpha(\mathbf{r},t) = \tilde{y}_\alpha(\mathbf{k},t)\exp(i\mathbf{k}\cdot\mathbf{r}')\,, \tag{6}$$

where $\tilde{y}_\alpha(\mathbf{k},t)$ is the amplitude of a mode with wavelength, $2\pi/k$. To simplify the analysis and to focus on the instability, the following is restricted to the special case $k_z = k_x = 0$, i.e., spatial perturbations only along the velocity gradient. The linear equations for $\tilde{y}_\alpha(\mathbf{k},t)$ are then of the form

$$\partial_t \tilde{y}_\alpha(\mathbf{k},t) + M_{\alpha\beta}(a,\mathbf{k})\tilde{y}_\beta(\mathbf{k},t) = 0 \tag{7}$$

with

$$\mathrm{M}(a,\mathbf{k}) = \begin{bmatrix} 0 & 0 & 0 & nik & 0 \\ c_1a^2 & (\eta/2e)a^2 + Dk^2 & -(2\eta T/e)aik & (pT/e)ik & 0 \\ -\nu_n aik & -(\nu/2T)aik & \nu k^2 & a & 0 \\ (p_n/\rho)ik & (p/\rho T)ik & 0 & \gamma k^2 & 0 \\ 0 & 0 & 0 & 0 & \nu k^2 \end{bmatrix}, \tag{8}$$

where $c_1 \equiv -\rho\nu_n T/e$, $D \equiv \lambda T/e$, $\nu \equiv \eta/\rho$, $\gamma \equiv \frac{4}{3}\nu + \kappa/\rho$, and $z_n \equiv \partial z/\partial n$.

The dispersion relations obtained from $\det(s\mathrm{I} - \mathrm{M}) = 0$ give five hydrodynamic modes, $s_\alpha(a,\mathbf{k})$. If the real parts of one or more modes become negative for some values of k and a then solutions to Eq. (7) grow in time, and the uniform shear flow state is linearly unstable. Direct calculation shows this is the case for sufficiently small k for any fixed and finite a. The hydrodynamic modes for finite a and asymptotically small k can be calculated explicitly to order k^2. Four modes vanish as $k \to 0$ while one is finite,

$$s_0 \to \nu k^2, \quad s_1 \to (\eta/2e)a^2, \quad s_2 \to c_2 k^2, \tag{9}$$

$$s_3 = s_4^* \to ick - (d_1 - d_2a^2)(k/a)^2, \tag{10}$$

where $\rho c^2 = [2p(2 + n\nu_n/\nu) + np_n]$, $\rho c^2 c_2 = n(3\nu p_n - 2p\nu_n)$, $(\rho\nu)^2 d_1 = p[2e(2\nu + n\nu_n) - \nu p]$, and $2d_2 = (3\nu + \gamma - c_2)$. These are positive constants depending only on the density and temperature of the reference state. The first three modes are stable, whereas the complex conjugate pair s_3 and s_4 are unstable for $a^2 < d_1/d_2$. *This is a primary observation of our work*: Within the limitations of the well-established Navier-Stokes equations (e.g., small k and small a) the equations are unstable for a reference state with sufficiently small shear rate. Conversely, a similar expansion of the eigenvalues in powers of a at fixed k shows the instability at all shear rates for sufficiently small k. These asymptotic results are confirmed by an exact evaluation of the eigenvalues from (8), using the Percus-Yevick approximation for the virial equation of state [11] and

using the Enskog kinetic theory to specify transport coefficients [12]. The results are shown in Fig. 1, indicating the line in the k-a plane separating stable (above) from unstable (below) dynamics at three different densities ($n^* \equiv n\sigma^3$, where σ is the hard sphere diameter). The instability is qualitatively the same for all densities.

The Navier-Stokes approximation for the heat and momentum fluxes requires $k \ll$ inverse mean free path and $a \ll$ inverse mean free time. Since the reference state is generated by the shear, it is possible that higher order contributions in a might remove the long wavelength instability. To address this question, it would be desirable to derive the linear hydrodynamic equations from the Boltzmann-Enskog kinetic equation without this limitation to small a. However, no solution to this kinetic equation is known, for either the reference uniform shear flow state or deviations from it. Consequently, we consider the case of low density for which the Boltzmann equation applies. While no solutions to this kinetic equation are known either, it is well established that closely related "kinetic models" provide practical and accurate representations of solutions to the Boltzmann equation. Here, we chose the nonlinear Bhatnagar-Gross-Krook (BGK) kinetic model obtained by replacing the Boltzmann collision operator with an average collision frequency, times the deviation of the distribution function from a local equilibrium distribution. The parameters of this local equilibrium distribution are chosen to enforce the exact conservation laws. As a consequence, the Navier-Stokes hydrodynamic equations obtained from the BGK model are the same as those from the Boltzmann equation—only the values of the transport coefficients differ. On this basis, we expect that hydrodynamic equations outside the Navier-Stokes limit derived from the BGK model should provide a faithful representation of those that would be obtained from the Boltzmann equation. These expectations for the BGK model have been confirmed in the case of shear flow by both analytical and numerical comparisons with the Boltzmann equation [13]. It is remarkable that the BGK equation can be solved exactly to determine the reference state distribution function for uniform shear flow, at arbitrary shear rate [14]. Using this known result, the heat and momentum fluxes in the conservation laws (1)–(3) can be determined to leading order in the deviations of the hydrodynamic fields from uniform shear flow. The resulting hydrodynamic equations linearized about the reference state are again valid only to order k^2, but now there is no *a priori* restriction on the value of the shear rate; the form of Eq. (7) is unchanged, but the matrix elements of $M_{\alpha\beta}(a, \mathbf{k})$ are not restricted to order a^2. This new shear rate dependence leads to qualitative differences from the Navier-Stokes equations (e.g., rheological effects such as shear thinning, normal stresses). The single parameter of this kinetic model is the average collision rate for the Boltzmann equation, and all dependence on the interaction potential occurs only through the temperature dependence of this parameter. We have chosen the simplest case of Maxwell molecules, $V(r) \sim r^{-4}$, for which it is a constant. All transport coefficients of these generalized linear hydrodynamic equations can be calculated exactly as functions of the shear rate, and the eigenvalues of $M_{\alpha\beta}(a, \mathbf{k})$ can be determined just as in the case of the Navier-Stokes equations. A long wavelength instability for any value of the shear rate is found again, now including values of a well outside the limitations of the Navier-Stokes equation, cf. Fig. 1. We conclude that the instability observed in (10) is robust and is not an aberration resulting from the approximations (4) and (5).

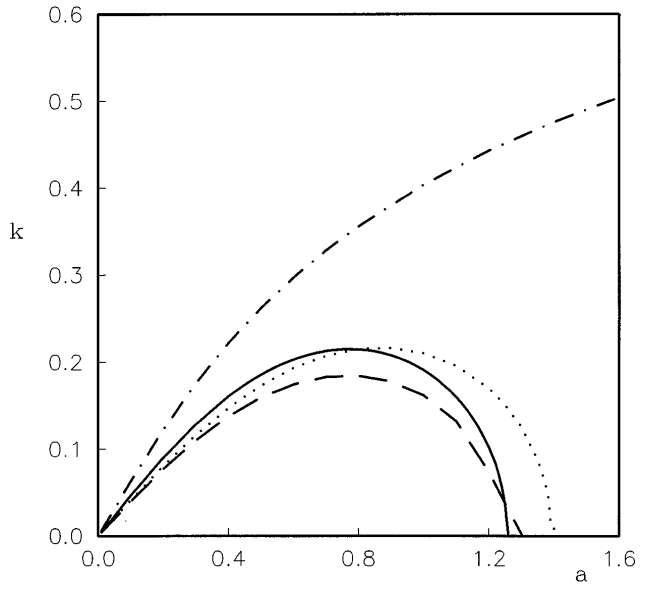

FIG. 1. Critical lines for stability determined from Eq. (8) at $n^* = 0$ (solid curve), $n^* = 0.2$ (dotted curve), and $n^* = 0.4$ (dashed curve). Also shown are the results from the BGK kinetic model for $n^* = 0$ (dash-dotted curve). All are in units of the mean free path and mean free time.

The extension of the hydrodynamic equations to larger shear rates using the BGK model allows comparison with Bird's direct simulation Monte Carlo method [6,15]. There have been significant tests of this method for uniform shear flow [13]. The method is so accurate and efficient that virtually all practical applications of gas kinetic theory far from equilibrium now use it. We have used a direct numerical solution to the BGK kinetic equation to test the stability analysis without the intermediate step of constructing a hydrodynamic description. The solution is constructed as follows. First, the volume is partitioned into cells, and N particles are distributed with positions and velocities according to a specified initial distribution. Next, at each finite time step $\tau <$ mean free time, a streaming and collision stage are computed. The particles are moved in straight lines to new positions at time $t + \tau$. For each particle, the probability of a collision is determined as the (local) collision frequency times τ. If a collision occurs, the velocity is replaced by a random velocity sampled from the local equilibrium distribution. This collision

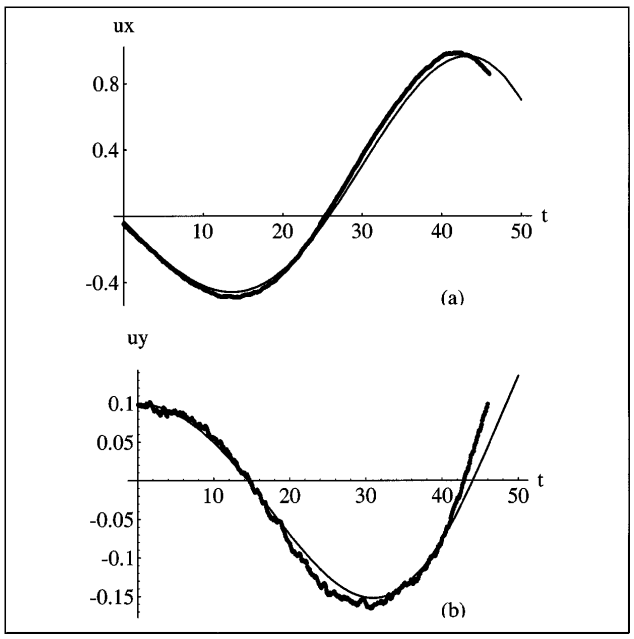

FIG. 2. Time evolution of (a) $\delta U_x(t)$ and (b) $\delta U_y(t)$ for $a = 0.5$ and $k = 0.1$ in units of the inverse mean free time and mean free path.

calculation is performed for all particles, and the whole process is iterated for many time steps.

To confirm our hydrodynamic analysis of the instability based on the BGK equations, an initial state for the hydrodynamic variables is chosen with $k = 0.1$ and $a = 0.5$ (in units of the inverse mean free path and time, respectively). This corresponds to conditions for which the linear hydrodynamic equations are unstable. The two unstable modes have complex eigenvalues so they lead to an oscillatory time dependence with growing amplitude. The hydrodynamic fields are constructed directly from an expansion in the eigenvectors of $M_{\alpha\beta}(a, \mathbf{k})$. To illustrate this dynamics we have chosen initial conditions such that $\delta U_y(0)$ couples only to the unstable modes, while $\delta U_x(0)$ couples to both stable and unstable modes. Figure 2 shows a comparison of the results for $\delta U_x(t)$ and $\delta U_y(t)$ as a function of time with those obtained from a Monte Carlo simulation of the BGK kinetic equation using the Bird method. The good agreement shows that the instability is not a consequence of the assumptions behind the hydrodynamic calculations, and also that these equations provide an accurate description of the initial stages of the instability. We have performed the simulations for times an order of magnitude longer than that shown. The maxima and minima continue to grow, although differences between the theory and simulation become more significant. This is expected since the linear hydrodynamic analysis is limited to small amplitudes.

It remains to understand the consequences of this long wavelength instability. We plan to extend the low density Monte Carlo simulations to very long times to see if a final stationary state is regained. At high densities, molecular dynamics simulations appear to be stable, except at very large shear rates where a transition to an ordered state occurs [9]. It is likely that the long wavelength instability considered here has not been seen due to the finite system sizes considered, i.e., $k > 2\pi/L$ [16]. We plan to explore longer wavelengths at high densities using both molecular dynamics and an extension of the Bird method to the dense fluid Enskog equation [17].

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[1] A. Lees and S. Edwards, J. Phys. C **5**, 1921 (1972).
[2] J. W. Dufty, J. J. Brey, and A. Santos in *Molecular Dynamics Simulation of Statistical Mechanical Systems*, edited by G. Ciccotti and W. G. Hoover (North-Holland, Amsterdam, 1986), pp. 295–303.
[3] J. W. Dufty, A. Santos, J. J. Brey, and R. Rodríguez, Phys. Rev. A **33**, 459 (1986).
[4] J. J. Brey, A. Santos, and J. W. Dufty, Phys. Rev. A **36**, 2842 (1987).
[5] *Nonlinear Fluid Dynamics*, edited by H. Hanley (North-Holland, Amsterdam, 1983).
[6] *Microscopic Simulation of Complex Flows*, edited by M. Mareschal (Plenum Press, New York, 1990).
[7] D. J. Evans and A. Baranyai, Phys. Rev. Lett. **67**, 2597 (1991); J. J. Brey, A. Santos, and V. Garzó, Phys. Rev. Lett. **70**, 2730 (1993).
[8] D. J. Evans, E. G. D. Cohen, and G. P. Morriss, Phys. Rev. A **42**, 5990 (1990).
[9] J. Erpenbeck, Phys. Rev. Lett. **52**, 1333 (1984).
[10] J. A. McLennan, *Introduction to Nonequilibrium Statistical Mechanics* (Prentice-Hall, Englewood Cliffs, NJ, 1989).
[11] J. P. Hansen and I. McDonald, *Theory of Simple Liquids* (Academic, New York, 1986), 2nd ed.
[12] J. H. Ferziger and H. G. Kaper, *Mathematical Theory of Transport Processes in Gases* (North-Holland, Amsterdam, 1972).
[13] J. M. Montanero and A. Santos, in *Rarefied Gas Dynamics 19*, edited by J. Harvey and G. Lord (Oxford University Press, Oxford, 1995); V. Garzó and A. Santos, Physica (Amsterdam) **213A**, 426 (1995); J. Gómez Ordóñez, J. J. Brey, and A. Santos, Phys. Rev. A **39**, 3038 (1989); **41**, 810 (1990).
[14] A. Santos and J. J. Brey, Physica (Amsterdam) **174A**, 355 (1991).
[15] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Clarendon Press, Oxford, 1994).
[16] J. M. Montanero, A. Santos, and V. Garzó, Phys. Lett. A **203**, 73 (1995).
[17] J. M. Montanero and A. Santos (to be published).