

Some Theoretical Aspects of Nonequilibrium Simulation Methods.

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1. - Introduction.

Many recent developments for systems far from equilibrium have resulted from novel methods for nonequilibrium computer simulation [1]. However, a direct comparison with theoretical predictions or experimental results has often been inconclusive, due to an imprecise correspondence to the numerical algorithms [2]. For example, the transport properties of a fluid under shear have been studied using standard molecular-dynamics techniques, except with periodic boundary conditions imposed in the Lagrangian frame for uniform shear flow. These are the Lees-Edwards boundary conditions [3], and they result in the desired macroscopic nonequilibrium flow field. However, in contrast to a real fluid sheared by mechanical contact with moving surfaces, the system heats up monotonically at spatially constant temperature and density. Thus, although the macroscopic velocity field is the same as that expected in an experimental situation, the other hydrodynamic fields differ and it is possible that the transport properties would also be different. In addition, external nonconservative forces can be used in the computer simulations to compensate for the viscous heating. This has the advantage of allowing for a stationary state, but it further complicates the relationship of transport properties obtained from such simulations to either experimental properties or those computed from theoretical models. The objective here is to summarize briefly a theoretical formulation of the Lees-Edwards type of simulation method and some results comparing shear viscosities for systems with and without viscous heating.

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2. - Nonequilibrium statistical mechanics.

A simple fluid of N particles in a cube of volume $V = (2l)^3$ is considered. The state of the system is characterized by a distribution function, $\varrho(\Gamma, t)$, defined over this region, where the phase point, $\Gamma = \{\mathbf{q}_\alpha, \mathbf{p}_\alpha\}$, denotes the positions and momenta in an inertial frame (the laboratory frame). The average of an observable, $A(\Gamma)$, is defined by

$$(1) \quad \langle A; t \rangle = \int d\Gamma A(\Gamma) \varrho(\Gamma, t).$$

The time dependence of the distribution function is calculated from the Liouville equation,

$$(2) \quad \left(\frac{\partial}{\partial t} + L \right) \varrho(\Gamma, t) + \sum_{\alpha} \nabla_{\mathbf{p}_\alpha} \cdot (\mathbf{f}_\alpha \varrho) = 0,$$

where L is the Liouville operator associated with the Hamiltonian, H , for the N particles,

$$(3) \quad L = \sum_{\alpha} \left[\frac{\mathbf{p}_\alpha}{m} \cdot \nabla_{\mathbf{q}_\alpha} + \sum_{\beta \neq \alpha} \mathbf{F}(\mathbf{q}_{\alpha\beta}) \cdot \nabla_{\mathbf{p}_\alpha} \right],$$

and $\mathbf{F}(\mathbf{q}_{\alpha\beta})$ is the force on the α -th particle due to the β -th particle (assumed to depend only on their relative separation, $\mathbf{q}_{\alpha\beta} = \mathbf{q}_\alpha - \mathbf{q}_\beta$). The last term on the left-hand side of eq. (2) represents the effects of a nonconservative force, \mathbf{f}_α , which in general is a function of the momenta. Equation (2) must be supplemented with suitable initial and boundary conditions. A general class of boundary conditions for the Liouville equation has the homogeneous form [4]

$$(4) \quad [\varrho(\Gamma, t)]_{\substack{\mathbf{q}_\alpha \in \Sigma \\ \mathbf{p}_\alpha \cdot \hat{n} > 0}} = \int_{\substack{\mathbf{q}'_\alpha \in \Sigma \\ \mathbf{p}'_\alpha \cdot \hat{n}' < 0}} d\Gamma' W(\Gamma, \Gamma'; t) \varrho(\Gamma', t),$$

where Σ is the surface for the volume and \hat{n} is a unit vector normal to the surface, directed inward. The function $W(\Gamma, \Gamma'; t)$ characterizes the distribution of particles entering the system in terms of those incident on the surface.

The system to be modelled is a fluid with equal but opposite average flow velocity at the surfaces $y = \pm l$. The average velocity field, $\mathbf{U}(\mathbf{r})$, is expected to be linear between these surfaces, and directed along the x -axis, *i.e.*

$$(5) \quad U_i(\mathbf{r}) = a_{ij} r_j, \quad a_{ij} = a \delta_{ix} \delta_{jy}.$$

Here, $a = \partial U_x / \partial y$ is the magnitude of the shear rate. For such a macroscopic flow it is useful to refer the positions and momenta of all particles to a frame of reference that is locally at rest with respect to the average flow. This is accomplished by a local Galilean transformation

$$(6) \quad \tilde{q}_{\alpha i} = \Lambda_{ij}(t) q_{\alpha j}, \quad \tilde{p}_{\alpha i} = p_{\alpha i} - m U_i(\mathbf{q}_\alpha), \quad \Lambda_{ij}(t) = \delta_{ij} - a_{ij} t.$$

The co-ordinate transformation is that for the Lagrangian variables of the flow. The Lees-Edwards boundary conditions are easily stated in terms of these variables: a particle incident on a surface at position $\tilde{\mathbf{q}}_\alpha$ with momentum $\tilde{\mathbf{p}}_\alpha$ is replaced by a particle on the opposite surface with the same momentum and same values for the co-ordinates within the surface. This prescription is consistent with a periodic extension of the original volume, and this extension is also part of the Lees-Edwards conditions. It is clear that these are the usual periodic boundary conditions for equilibrium simulations, except that they are applied in the rest frame.

The above can be translated into corresponding boundary conditions for the Liouville equation. Using the notation $\tilde{G}(\tilde{\Gamma}) = G(\Gamma)$ for the transformation of an arbitrary function, G , under (6) (where $\tilde{\Gamma} = \{\tilde{\mathbf{q}}_\alpha, \tilde{\mathbf{p}}_\alpha\}$), the Lees-Edwards boundary conditions in terms of eq. (4) are

$$(7) \quad \tilde{W}(\tilde{\Gamma}, \tilde{\Gamma}') = \delta(\tilde{\mathbf{p}}_\alpha - \tilde{\mathbf{p}}'_\alpha) \delta(\tilde{q}_{\alpha z} + \tilde{q}'_{\alpha z}) \delta(\tilde{q}_{\alpha y} - \tilde{q}'_{\alpha y}) \delta(\tilde{q}_{\alpha x} - \tilde{q}'_{\alpha x}) \cdot \prod_{\beta \neq \alpha} \delta(\tilde{\mathbf{q}}_\beta - \tilde{\mathbf{q}}'_\beta) \delta(\tilde{\mathbf{p}}_\beta - \tilde{\mathbf{p}}'_\beta),$$

for $\tilde{q}_{\alpha z} = \pm l$ and $\tilde{\mathbf{q}}_\beta \notin \Sigma$ for $\beta \neq \alpha$. Similar expressions apply for $\tilde{q}_{\alpha y} = \pm l$ and $\tilde{q}_{\alpha x} = \pm l$, and the generalization to many particles simultaneously on the surface is straightforward. Equations (6) and (7) lead to the simpler condition

$$(8) \quad [\tilde{\rho}(\tilde{\Gamma}, t)]_{\tilde{q}_{\alpha z}=l} = [\tilde{\rho}(\tilde{\Gamma}, t)]_{\tilde{q}_{\alpha z}=-l},$$

so that the distribution function on opposite surfaces must be the same. Equation (8) is also compatible with a periodic extension of the original volume, but it is necessary to show that the Liouville equation will admit such periodic solutions. In the rest frame variables eqs. (2) and (3) become

$$(9) \quad \begin{cases} \left(\frac{\partial}{\partial t} + \mathcal{L} \right) \tilde{\rho} + \sum_{\alpha} \nabla_{\tilde{\mathbf{v}}_\alpha} \cdot (\tilde{\mathbf{f}}_\alpha \tilde{\rho}) = 0, \\ \mathcal{L} = \sum_{\alpha} \left[\Lambda_{ij}(t) \frac{\tilde{p}_{\alpha j}}{m} \frac{\partial}{\partial \tilde{q}_{\alpha i}} - a_{ij} \tilde{p}_{\alpha j} \frac{\partial}{\partial \tilde{p}_{\alpha i}} + \sum_{\beta \neq \alpha} \tilde{\mathbf{F}}(\tilde{\Lambda}(-t) \cdot \tilde{\mathbf{q}}_{\alpha\beta}) \cdot \nabla_{\tilde{\mathbf{v}}_\alpha} \right]. \end{cases}$$

The Liouville equation in these variables is, therefore, invariant under co-ordinate translations, if the nonconservative force is invariant. A sufficient condi-

tion for periodic solutions is a periodic representation of the conservative and nonconservative forces, and the boundary condition (8). For self-consistency, the class of observables in (1) should also be given a periodic extension. Equations (1), (8) and (9) constitute the statistical mechanical formulation of the Lees-Edwards boundary-value problem.

A class of homogeneous solutions to (9) results for initial conditions, $\tilde{q}(\vec{r}, t = 0)$, that are translationally invariant functions. In that case the macroscopic conservation laws are satisfied by an average number density, momentum density and energy density given by

$$(10) \quad \begin{cases} \langle n(\mathbf{r}); t \rangle = n_0, & \langle \mathbf{p}(\mathbf{r}); t \rangle = n_0 m \mathbf{U}(\mathbf{r}), \\ \langle u(\mathbf{r}); t \rangle = \frac{1}{2} m n_0 \mathbf{U}^2(\mathbf{r}) + \varepsilon(t). \end{cases}$$

Here, m is the mass, $\mathbf{U}(\mathbf{r})$ is the flow field (5), n_0 is the constant density, and $\varepsilon(t)$ is the internal energy, whose time evolution is governed by

$$(11) \quad \frac{\partial}{\partial t} \varepsilon(t) = - a_{ij} P_{ij} + V^{-1} \langle \sum_{\alpha} \mathbf{f}_{\alpha} \cdot \mathbf{p}_{\alpha}; t \rangle,$$

where P_{ij} is the average pressure tensor (defined below). Equations (10) and (11) include the additional constraints of zero average nonconservative force and initial momentum. The macroscopic hydrodynamic equations, therefore, have exactly the flow field desired, and spatially uniform internal energy and density. Interestingly, these results are exact for all \mathbf{r} and t ; there are no boundary layers, and all initial transients occur only through $\varepsilon(t)$. This is a very special feature of the Lees-Edwards boundary conditions.

The transport properties characterize the pressure tensor as a function of the shear rate and $\varepsilon(t)$. At small shear rates Newton's viscosity law is expected to hold, $P_{ij} = p \delta_{ij} - \eta_0 (a_{ij} + a_{ji})$, where p is the hydrostatic pressure and η_0 is the shear viscosity. More generally, it follows from the symmetry of the problem that the pressure tensor has the form

$$(12) \quad P_{ij} = \left[p + \frac{a^2}{3} (\psi_1(a) + 2\psi_2(a)) \right] \delta_{ij} - \eta(a) (a_{ij} + a_{ji}) - \psi_1(a) a_{ik} a_{jk} - \psi_2(a) (a_{ik} a_{jk} + a_{ki} a_{kj}).$$

The three scalar functions are the nonlinear shear viscosity, $\eta(a)$, and the first and second viscometric functions, $\psi_1(a)$ and $\psi_2(a)$, respectively. The pressure tensor can be calculated from

$$(13) \quad \begin{cases} P_{ij} = V^{-1} \langle T'_{ij}; t \rangle, \\ T'_{ij} = \sum_{\alpha} \left[\frac{1}{m} \tilde{p}_{\alpha i} \tilde{p}_{\alpha j} + \frac{1}{2} \sum_{\beta \neq \alpha} q_{\alpha \beta i} F_j(\mathbf{q}_{\alpha \beta}) \right]. \end{cases}$$

(The phase function, T'_{ij} , is that part of the microscopic stress tensor excluding convection by the macroscopic flow.)

The objective now is to obtain useful representations of the pressure tensor from formal solutions to the Liouville equation. The transport properties vanish in the local equilibrium ensemble, so it is useful to represent formal solutions in terms of the deviation from this ensemble,

$$(14) \quad \tilde{q}(t) = \tilde{q}_L(t) + \tilde{A}(t), \quad \tilde{q}_L(t) = \exp[-\beta(t)\tilde{H}'] / \int d\tilde{\Gamma} \exp[-\beta(t)\tilde{H}'],$$

where $H' = H(\{\mathbf{q}_\alpha, \tilde{\mathbf{p}}_\alpha\})$, *i.e.* it is the Hamiltonian for the system, but with the laboratory momentum replaced by the rest frame momentum. This simple form of the local equilibrium ensemble is another special aspect of the hydrodynamic field (10), resulting from the Lees-Edwards boundary conditions. The parameter $\beta(t)$ is defined by the requirement

$$(15) \quad \langle H'; t \rangle = \langle H' \rangle_{\beta(t)} \equiv \int d\tilde{\Gamma} \tilde{q}_L(t) \tilde{H}'.$$

It follows that $T(t) = (k_B \beta(t))^{-1}$ is a nonequilibrium temperature whose functional relationship to the internal energy is the same as that in equilibrium. This is distinguished from the kinetic temperature, $T_k(t) = 2\langle K'; t \rangle / 3k_B N$, where $K' \equiv \sum_\alpha (\tilde{p}_\alpha^2 / 2m)$ is the kinetic energy relative to the flow. A formal expression for $\tilde{A}(t)$ is obtained from the Liouville equation (with $\tilde{A}(t=0) = 0$),

$$(16) \quad \begin{cases} \tilde{A}(t) = - \int_0^t d\tau \tilde{\mathcal{U}}(t, \tau) S(\tau) \tilde{q}_L(\tau), \\ S(t) = \beta(t) a_{ij} T'_{ij} - \frac{\partial \beta(t)}{\partial t} (\tilde{H}' - \langle \tilde{H}' \rangle_{\beta(t)}) - \sum_\alpha \left(\beta(t) \tilde{\mathbf{f}}_\alpha \cdot \frac{\tilde{\mathbf{p}}_\alpha}{m} - \nabla_{\tilde{\mathbf{x}}_\alpha} \cdot \tilde{\mathbf{f}}_\alpha \right), \end{cases}$$

where $\tilde{\mathcal{U}}(t, z)$ is the solution operator for the Liouville equation,

$$(17) \quad \left(\frac{\partial}{\partial t} + \mathcal{L} \right) \tilde{\mathcal{U}}(t, \tau) + \sum_\alpha \nabla_{\tilde{\mathbf{x}}_\alpha} \cdot \tilde{\mathbf{f}}_\alpha \tilde{\mathcal{U}}(t, \tau) = 0, \quad \tilde{\mathcal{U}}(\tau, \tau) = 1.$$

The function $S(t)$ represents three types of sources for the nonequilibrium state. The first arises from the inertial forces due to the Lees-Edwards boundary conditions imposed in a noninertial frame. The second term is an effect of the viscous heating, and the third is entirely associated with the nonconservative force.

In the following, attention will be restricted to the shear viscosity. From

eqs. (12)-(16), this is given by

$$(18) \quad a\eta(a, t) = \int_0^t d\tau V^{-1} \langle T'_{xy}(t, \tau) S(\tau) \rangle_\beta,$$

where the time dependence has been shifted to $T'_{ij}(t, \tau) = \tilde{\mathcal{U}}^\dagger(t, \tau) T'_{ij}$, and $\tilde{\mathcal{U}}^\dagger$ denotes the adjoint of $\tilde{\mathcal{U}}$. In the next section this expression is considered in more detail for two specific choices for the nonconservative force.

3. - Constant-temperature shear viscosity.

One important reason for introducing the nonconservative force is to control viscous heating. As mentioned in the introduction, it is not clear what other effects are induced in the system when such forces are effective. Here, the shear viscosity at constant temperature is compared with that for a system with only the conservative Newtonian force. It should be noted at the outset that the nonconservative force used to hold the temperature constant is not unique, and a choice of convenience is made here to allow for a rather detailed analysis in the low-density limit. Further comment on this point is made in the discussion section.

The form for the nonconservative force commonly used in computer simulations is a « drag » force,

$$(19) \quad \tilde{f}_\alpha = -\lambda \tilde{p}_\alpha,$$

where λ can be selected to control the temperature $T(t)$ (or some other property of the system). For constant temperature the condition is

$$(20) \quad \frac{\partial \varepsilon(t)}{\partial t} = -V^{-1} \langle [2\lambda K' + a_{ij} T'_{ij}]; t \rangle = 0,$$

which is satisfied by

$$(21) \quad \lambda = -a_{ij} \langle T'_{ij}; t \rangle / \langle 2K'; t \rangle = a^2 \eta(a, t) / 2\varepsilon_k(t).$$

The second equality follows from the definition of the shear viscosity in eqs. (12) and (13), and $\varepsilon_k(t) = V^{-1} \langle K'; t \rangle$. The formal expressions for the nonlinear shear viscosities with and without nonconservative forces can now be compared. These viscosities are denoted by $\eta^{(i)}(a, t)$, with $i = 1$ for the case of viscous heating ($\lambda = 0$) and $i = 2$ for constant temperature (λ given by eq. (21)). From (18) a common form for the expressions is obtained,

$$(22) \quad \eta^{(i)}(a, t) = \int_0^t d\tau [C(t, \tau | \beta(\tau)) - a\eta^{(i)}(a, \tau) D^{(i)}(t, \tau | \beta(\tau))],$$

where $C(t, \tau|\beta(\tau))$ and $D^{(i)}(t, \tau|\beta(\tau))$ are the correlation functions,

$$(23) \quad \left\{ \begin{array}{l} C(t, \tau|\beta(\tau)) \equiv \beta(\tau) V^{-1} \langle T'_{xy}(t, \tau) T'_{xy} \rangle_{\beta(\tau)}, \\ D^{(1)}(t, \tau|\beta(\tau)) \equiv \frac{\partial \beta(\tau)}{\partial \varepsilon(\tau)} V^{-1} \langle T'_{xy}(t, \tau) [\tilde{H}' - \langle \tilde{H}' \rangle_{\beta(\tau)}] \rangle_{\beta(\tau)}, \\ D^{(2)}(t, \tau|\beta) \equiv \frac{\partial \beta_{\mathbf{k}}(\tau)}{\partial \varepsilon_{\mathbf{k}}(\tau)} V^{-1} \left\langle T'_{xy}(t, \tau) \left[\frac{\beta}{\beta_{\mathbf{k}}(\tau)} \tilde{K}' - \langle \tilde{K}' \rangle_{\tau} \right] \right\rangle_{\beta}. \end{array} \right.$$

It is understood here that the time dependence of $T'_{ij}(t, \tau)$ in these expressions is calculated using the appropriate λ for each case.

The forms of the shear viscosities for the two cases are seen to be quite similar. In the first, $T(t)$ varies in time, while, in the second, $T(t)$ is constant but $T_{\mathbf{k}}(t)$ varies. Further considerations show that $D^{(2)}$ differs in form from $D^{(1)}$ only by fluctuations in the potential energy. Consequently, the structure of the shear viscosities is the same in the low-density limit, with only $T(t)$ and λ being different. Also, since $T_{\mathbf{k}}(t) \rightarrow T(t) = \text{const}$ at low density in case 2, a stationary value for $\eta^{(2)}(a, t)$ may be expected. At finite density a stationary value is apparently not obtained, even though the hydrodynamic state variables are constant in time. In the Navier-Stokes limit the second term in the brackets of eq. (22) vanishes, the temperature becomes constant, and the time evolution of $T'_{xy}(t, \tau)$ is Newtonian with periodic boundary conditions in the laboratory frame. Consequently, both cases 1 and 2 agree with the Green-Kubo result in this limit.

Equations (22) are highly nonlocal and nonlinear. Nevertheless, a closed description of the transport properties at the macroscopic level is obtained once the correlation functions have been determined, which may prove useful for approximations at large shear rates. For example, at low density it can be shown [5] that the correlation functions are determined from a bilinear kinetic equation related to the nonlinear Boltzmann equation (the method of ref. [5] extends in a straightforward way to include the nonconservative force chosen here). The resulting shear viscosities are also equivalent to those obtained directly from the kinetic-theory pressure tensor,

$$(24) \quad P_{ij}(t) = \int d\tilde{\mathbf{p}} \frac{1}{m} \tilde{p}_i \tilde{p}_j \tilde{f},$$

where \tilde{f} is the homogeneous solution to the nonlinear Boltzmann equation in the local rest frame,

$$(25) \quad \left[\frac{\partial}{\partial t} - a_{ij} \tilde{p}_j \frac{\partial}{\partial \tilde{p}_i} - \lambda \nabla_{\tilde{\mathbf{v}}} \cdot \tilde{\mathbf{p}} \right] \tilde{f} = J[\tilde{f}, \tilde{f}].$$

Use has been made of Lees-Edwards boundary conditions at low density [6]

and invariance of the collision operator under transformation to the rest frame. Finally, λ in (25) is given by the low-density limit of (21) for case 2, or zero for case 1. In the latter case, IKENBERRY and TRUESDELL [7] have calculated the exact nonlinear shear viscosity from (24) and (25) for Maxwell molecules ($F(q) \sim q^{-5}$). The method can be applied to case 2 as well, so that the shear viscosities are known in detail for all values of the shear rate at low densities. To state the result, a dimensionless shear rate, $\bar{a} = a/\nu$, and shear viscosity, $\bar{\eta}(\bar{a}) = \eta(a)\nu/p$, are introduced. Here ν is a constant associated with an eigenvalue of the collision operator. The result for Maxwell molecules is then

$$(26) \quad \bar{\eta}^{(1)}(\bar{a}) = \bar{\eta}^{(2)}(\bar{a}).$$

This equivalence of constant-temperature and viscous-heating states extends to all other transport properties as well [6].

This is an encouraging result to support the view that the nonconservative forces are «passive», *i.e.* that the temperature can be controlled without affecting the transport properties. However, the exact equivalence for Maxwell molecules probably holds only at low density, and cannot be extended to other force laws even in this limit. To support this latter statement, the shear viscosity has been determined for a class of force laws, $F \sim q^{-n}$, for a model of the nonlinear Boltzmann equation (the BGK model) [8]. For $n = 5$ the model gives the same viscosities as the Boltzmann equation and (26) is regained. For $n \neq 5$ the equality in (26) fails, so that different transport properties are obtained when the viscous heating is controlled. In the case of hard spheres ($n \rightarrow \infty$) the coefficients of order \bar{a}^2 in the shear viscosity (super Burnett coefficients) differ by about 30%. However, the functions $\bar{\eta}^{(1)}(\bar{a})$ and $\bar{\eta}^{(2)}(\bar{a})$ are quite similar over the whole range of shear rates, with a maximum difference of about 16%.

4. - Discussion.

Two main topics have been addressed here: a suitable formulation of the Lees-Edwards boundary-value problem and the influence of nonconservative forces on transport properties. Regarding the first, the Liouville equation (9) with periodic boundary conditions, (8), is appropriate for the calculation of transport and other properties (*e.g.*, structure factors, fluctuations) for both homogeneous and inhomogeneous states. It is also the form suitable for comparison with a class of computer simulations. The effects of nonconservative forces on transport properties are somewhat difficult to predict *a priori*. The example given here shows that it is possible to control the temperature by such forces without changing the qualitative behaviour of transport in the system, although it also indicates that quantitative differences are to be expected. Some additional points not addressed here should be noted:

a) The Lees-Edwards boundary conditions are nonlocal, relating the distribution on one surface to that on the opposite surface. As a consequence, there are no boundary layers or spatial variations in the temperature. At best it is an idealized representation of the bulk properties of real fluids. Some care is required in comparison with other computer simulation methods that are more realistic (*e.g.*, stochastic boundary condition methods [9]).

b) The periodic boundary conditions are applied in a noninertial frame, and there are «inertial forces» in the corresponding Newtonian equations of motion. The latter are equivalent to one of the «non-Newtonian» methods used in computer simulation (the Doll's tensor form [10] is apparently incorrect). Such methods are interpreted here as Newtonian, but expressed in the frame of reference for which the boundary conditions are simplest.

c) The nonconservative force chosen in sect. 3 is not unique. A stronger constraint is to hold the total microscopic energy constant in time. In that case the parameter λ becomes a phase function

$$(27) \quad \lambda = - a_{ij} T'_{ij} / 2K',$$

and the nonlinear shear viscosity is found to be

$$(28) \quad \eta(a) = \int_0^t d\tau V^{-1} \langle T'_{xy}(t, \tau) (3N/2K') T'_{xy} \rangle_{\beta}.$$

This is a particularly simple form, similar to the Green-Kubo result of linear response. However, in contrast to the force of sect. 3, eq. (27) implies an inherently many-body, nonlocal force. It does not appear possible to describe this case by kinetic theory, even in the low-density limit. While it is possible to show that the shear viscosity in the Navier-Stokes limit agrees with the Green-Kubo result (to order N^{-1}), no further connection with real fluids has been established.

d) A local form for λ can be found, consistent with constant microscopic energy, that avoids the theoretical problems of (27). However, the result differs from the Green-Kubo result even at Navier-Stokes order ($\sim 100\%$ at low density). This illustrates the need for a detailed analysis of each method chosen to control heating.

e) An alternative to controlling the total energy is to require constant kinetic energy. This is the usual method for nonequilibrium computer simulations. In this case, even the results at zero shear rate are uncertain (although the correct thermodynamics is obtained). Preliminary considerations indicate

that the Navier-Stokes order results are quite close to the Green-Kubo results [11].

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