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Viscoelastic effects from the Enskog equation for uniform shear flow

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The Enskog kinetic equation for hard spheres is the only tractable theory with which the transport properties of a moderately dense gas can be studied. However, relatively little is known about its solutions outside the linear regime. In this paper two approximate nonlinear solutions of the Enskog equation for uniform shear flow are presented: a perturbative solution to second order in the shear rate and to fourth order in velocity moments and a ''nonperturbative'' moment solution to all orders in the shear rate and to second order in the velocity moments. A comparison to the results of nonequilibrium molecular-dynamics simulations shows that the perturbative results give good estimates of the quadratic corrections to the pressure tensor while the nonperturbative solution gives a semiquantitative description of viscoelastic effects including shear thinning and the normal stresses over a wide range of shear rates. The relevance of these results to the construction of kinetic models of the Enskog equation is also discussed. [S1063-651X(97)08512-7]

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I. INTRODUCTION

The Enskog equation, describing the time evolution of the one-body distribution function for hard spheres, is the only tractable and realistic kinetic equation for a moderately dense system [1–3]. It was originally proposed on physical grounds as a heuristic generalization of the Boltzmann equation and has since been further extended by van Beijeren and Ernst [4] to give a unified basis for the description of fluid, solid, and metastable states [5]. Near equilibrium, the standard method for analyzing all of these models, since they are structurally very similar, is the Chapman-Enskog expansion. At lowest nontrivial order, this gives explicit expressions for the linear (Navier-Stokes order) transport coefficients in terms of the intermolecular potential. The Boltzmann-level results provide a good description of linear transport in a wide range of low-density gases and mixtures [2,3]. The Enskog results are well known for their surprising accuracy with, e.g., the shear viscosity of the hard-sphere gas being accurately predicted up to a density of one-half of the freezing point [6]. Higher-order terms in the expansion describe nonlinear transport. However, because of the intricate nature of the models, the expansion is analytically complex to carry through so that general results are only known to third order for the Boltzmann equation [2,7], while only part of the second- and third-order contributions have been calculated for the Enskog equation [8]. Apart from these perturbative results, only a handful of exact solutions are known and then only for the Boltzmann equation [9]. Thus, even with the Boltzmann equation, systems far from equilibrium can only be studied by numerical methods or by means of simplified versions of the model. Both of these methods have recently been extended to the Enskog equation [10,11], although neither has yet been widely studied.

The purpose of this paper is to give a picture of nonlinear transport as described by the Enskog theory for the particular case of a sheared fluid. The state of uniform shear flow (USF), in which the macroscopic flow velocity, defined to be along the x axis, varies linearly with position along an orthogonal axis, e.g., the y axis, has been the subject of numerous studies, both theoretical and by means of computer simulation [12]. Indeed, one of the rare exact solutions to the Boltzmann equation is that for a system of Maxwell molecules (interacting via an inverse fourth power potential) undergoing USF [13,14]. This focus of attention is largely due to the fact that USF can be established by the application of modified (Lees-Edwards) periodic boundaries [15], thus making it easy to simulate and incidently eliminate from theoretical analysis complicating features such as boundary layers associated with walls. Furthermore, the state of USF provides a direct probe of some of the transport properties of the fluid: For example, with the axes mentioned above, the x-y component of the stress tensor is the shear viscosity times the shear rate. A final motivation is the fact, discovered [16] about ten years ago, that at high shear rates simple fluids (including the hard-sphere fluid) undergo an ordering transition whereby the atoms are arranged in planes or strings perpendicular to the flow gradient. Indeed, two closely related Enskog-based theories of this transition have been formulated [17,18], which, although in qualitative agreement with the simulations, require as input the steady-state distribution at high shear rates for which the use of the perturbative results is questionable. The present work was motivated, in part, by a desire to investigate this point.

As mentioned above, the standard analysis of the Enskog equation makes use of the Chapman-Enskog expansion according to which the distribution is expanded in terms of a quantity characterizing the uniformity of the fluid: For USF this is simply the shear rate. This leads to a set of linear integral equations that are usually solved by means of the Chapman-Cowling expansion [2,3], which is an expansion in terms of a set of orthogonal polynomials of the momentum (the Sonine polynomials). The first expansion obviously limits the use of low-order results to small gradients, while the second expansion is devoid of physical content and is simply a mathematical convenience. An alternative method, first proposed by Grad [19,2,3,20,21] for analyzing the Boltz-

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mann equation, is to first expand the distribution (about local equilibrium) in terms of a complete set of orthogonal polynomials in the momentum. This, together with other simplifying assumptions, including the truncation of the expansion of the distribution, leads to a set of equations for the coefficients that are essentially an extension of the Navier-Stokes equations and that have been used to study the behavior of fluids under extreme conditions, e.g., in shock waves. Depending on the number of coefficients retained, Grad's original equations are known in the literature as the 13- or 20-moment approximations. More generally, the method consists in projecting the kinetic equation onto a finite-dimensional space spanned by the chosen basis functions, the choice of basis functions being restricted by the particular boundary conditions being imposed [21]. The moment approximation is interesting because no explicit assumption is made about the size of the gradients in the system: Although small gradients might provide a justification for truncating the expansion of the distribution function, it is not in general required. Indeed, all of the assumptions Grad made to derive his approximations are exact [20] for the Maxwell gas (inverse fourth power potential) undergoing USF described by the Boltzmann equation, which is in fact the reason that Ikenberry and Truesdell were able to solve the Boltzmann equation in this case. Thus the moment method has played a role in the study, e.g., of extended hydrodynamic modes [22] where assumptions about the size of inhomogeneities cannot be made. Here it is shown that the lowest nontrivial order of the moment expansion gives a quantitatively reasonable model for shear thinning and normal stresses at large shear rates. The discussion of this point is an extension of the preliminary account that appeared in Ref. [23].

In this paper the moment method is applied to the Enskog equation for a system undergoing USF and the solutions are compared to the results of molecular-dynamics simulations. In Sec. II the existence of a stationary solution under the conditions used to study USF by computer simulation is discussed and two calculations based on a moment expansion of the distribution are presented. The first is the complete solution to second order in the shear rate and to fourth order in the (velocity) moments. The second is the solution to second order in the moments and to all orders in the shear rate. These are compared, in Sec. III, to computer simulations for a relatively dense fluid and it is found that the accuracy of the Enskog equation appears to extend into the nonlinear regime with the perturbative results being numerically accurate near equilibrium and the nonperturbative results giving a semiquantitative description of the shear viscosity and normal stresses over the entire range of shear rates up to the ordering transition. The paper concludes in Sec. IV with an extended discussion of the implications of these results on the construction of a simple kinetic model of the Enskog equation and on the construction of a (model) positive-definite distribution function for strongly sheared hard-sphere fluids.

II. MOMENT SOLUTIONS TO THE ENSKOG EQUATION

Both the Enskog and the Boltzmann equations for the one-body reduced distribution function may be written as

$$\frac{\partial}{\partial t} f(\vec{q},\vec{v};t) + \vec{v}\cdot\frac{\partial}{\partial \vec{q}} f(\vec{q},\vec{v};t) + \frac{\partial}{\partial \vec{v}}\cdot \vec{F}_{ext}(\vec{q},\vec{v};t) f(\vec{q},\vec{v};t) = J[f,f], \tag{2.1}$$

where $\vec{q}$ and $\vec{v}$ are position and velocity and the difference between the Enskog and the Boltzmann equations lies in the form of the bilinear collision operator, which is given explicitly in Appendix A. The final term on the left-hand side is a possible contribution due to an externally imposed one-body force: Most studies of USF include such a force to maintain a constant temperature as described below. The equation must be supplemented by boundary conditions, which are taken to be the Lees-Edwards conditions used in computer simulations of sheared flow [15]. These are defined as periodic boundaries in the rest frame of the imposed flow profile. Specifically, if the desired flow is taken to be

$$\vec{v}_0(\vec{r}) = \overleftrightarrow{a}\cdot\,\vec{r} \equiv a y \hat{x} \tag{2.2}$$

in a Cartesian coordinate system with basis $(\hat{x},\hat{y},\hat{z})$, then the rest-frame coordinates are simply $\vec{q}\,' = \vec{q} - \vec{v}_0(\vec{q})t$ and $\vec{v}\,' = \vec{v} - \vec{v}_0(\vec{q})$ and periodic boundaries are imposed with respect to $\vec{q}\,'$. It is easy to verify that if the external force is only a function of $\vec{v}\,'$ then Eq. (2.1), expressed in the rest frame, is translationally invariant (for both the Boltzmann and Enskog collision operators) and since the boundary conditions are as well, the equation admits of spatially homogeneous solutions. More generally, the solution need only be periodic in the rest frame and, indeed, recent studies have indicated that USF may not be the stable state for large systems [24]. Our interest here, however, is to understand the properties of the relatively small systems studied by computer simulation and from which transport and viscoelastic properties may be measured and for these the homogeneous solution is of most interest. Given this, we seek solutions that are spatially homogeneous in the local rest frame. It simplifies matters to note that such solutions are also homogeneous when expressed in terms of the laboratory coordinates and excess velocity in which case we may write

$$f(\vec{q},\vec{v};t) = \tilde{f}(\vec{v}\,';t) \tag{2.3}$$

provided, of course, that the external force depends only on the excess velocity $\vec{v}\,'$ and time, which will henceforth be assumed to be true.

To specify the macroscopic state, one needs to know the hydrodynamic fields, the local density velocity, and energy density, or temperature, which are respectively defined as

$$\rho(\vec{q},t) = \int d\vec{v}\; f(\vec{q},\vec{v},t),$$

$$\rho(\vec{q},t)\vec{u}(\vec{q},t) = \int d\vec{v}\; \vec{v} f(\vec{q},\vec{v},t), \tag{2.4}$$

$$e(\vec{q},t) \equiv \frac{3}{2}\rho(\vec{q},t)k_B T(\vec{q},t) = \int d\vec{v}\frac{1}{2}[\vec{v}-\vec{u}(\vec{q},t)]^2 f(\vec{q},\vec{v},t),$$

and, in general, are also determined from the Enskog equation

$$\frac{\partial \rho}{\partial t}+\vec{\nabla}\cdot \rho \vec{u}=0,$$

$$\frac{\partial \rho \vec{u}}{\partial t}+\vec{\nabla}\cdot\langle \vec{v}\vec{v}\rangle=\langle \vec{v}\vec{F}_{ext}(\vec{q},\vec{v};t)\rangle+\int d\vec{v}\ \vec{v}J[f,f],$$

$$\frac{\partial}{\partial t}e(\vec{q},t)+\vec{\nabla}\cdot\left\langle \vec{v}\frac{1}{2}[\vec{v}-\vec{u}(\vec{q},t)]^2\right\rangle$$
$$=\langle \vec{F}_{ext}(\vec{q},\vec{v};t)\cdot[\vec{v}-\vec{u}(\vec{q},t)]\rangle$$
$$+\int d\vec{v}\frac{1}{2}[\vec{v}-\vec{u}(\vec{q},t)]^2 J[f,f], \tag{2.5}$$

where the angular brackets indicate an average over velocities. (Here and henceforth, the mass of the particles is taken to be one.) Given the form of the distribution (2.3), it immediately follows that the density is spatially homogeneous as is the excess velocity $\vec{u}(\vec{q},t)-\vec{v}_0(\vec{q})$, so that, if the center-of-mass position and velocity are taken to be zero, we have $\vec{u}(\vec{q},t)=\vec{v}_0(\vec{q})$. This then implies that $e(\vec{q},t)\equiv\langle\frac{1}{2}[\vec{v}-\vec{u}(\vec{q},t)]^2\rangle=\langle\frac{1}{2}(\vec{v}\,')^2\rangle$ is also spatially homogeneous and the conservation equations become

$$\frac{\partial \rho}{\partial t}=0,$$

$$\frac{\partial \rho \vec{u}}{\partial t}=0, \tag{2.6}$$

$$\frac{\partial}{\partial t}e(t)-a_{ij}\langle v_i' v_j'\rangle-\langle \vec{F}_{ext}(\vec{v}\,')\cdot\vec{v}\,'\rangle=\frac{1}{2}\int d\vec{v}\,'(\vec{v}\,')^2 J[f,f],$$

thus demonstrating that the macroscopic state is indeed that of uniform shear flow with a time-dependent temperature. In computer simulations, it is usual to include an external force to keep the temperature constant so as to establish a steady state. Although there are many possible choices of the external force [25], only the simplest, given by $\vec{F}_{ext}(\vec{v}\,')=\gamma\vec{v}\,'$, where γ is a constant, will be considered here. Stationarity of the energy then gives

$$-3(\rho k_B T)\gamma=a_{ij}\langle v_i' v_j'\rangle+\frac{1}{2}\int d\vec{v}\,'(\vec{v}\,')^2 J[f,f]\equiv a_{ij}P_{ij}, \tag{2.7}$$

where the last equality follows by comparing Eqs. (2.6) to the macroscopic conservation laws. With the present choice of coordinates [Eq. (2.2)], $a_{ij}=a\delta_{ix}\delta_{jy}$ and $-3(\rho k_B T)\gamma=aP_{xy}=-a^2\eta$, where η is the (shear-rate-dependent) shear viscosity.

The Enskog equation is usually solved by means of the Chapman-Enskog expansion [2,3], which, in the present case, is an expansion of the distribution in powers of the shear rate. The coefficients of the expansion in turn depend on the (scalar) momentum and must be expanded as well (usually in terms of Sonine polynomials). An alternative, proposed by Grad [2,19,20], is to first expand the distribution about the local-equilibrium distribution in terms of the momentum as

$$f(\vec{q},\vec{p},t)=\rho(\vec{q},t)\phi(\vec{c})\left\{1+\sum_{n=0}\frac{1}{n!}\varepsilon^n A_{[n]}P_{[n]}(\vec{c})\right\}, \tag{2.8}$$

where $\vec{c}=\sqrt{m/k_B T}\vec{v}\,'$ is a dimensionless excess velocity, $\phi(\vec{c})=(1/2\pi k_B T)^{3/2}e^{-c^2/2}$ is the local-equilibrium distribution, and ε is a fictitious parameter used to order the expansion. The functions $P_{[n]}(\vec{p})$ are a complete set of polynomials in the components of $\vec{p}$. The prefactor is chosen for later convenience and a short notation for multiple indices has been introduced whereby $A_{[n]}\equiv A_{i_1\cdots i_n}$ and repeated indices are summed. The series is truncated at some finite order in ε, to be specific, we keep all terms to order ε^k, and the $k-3$ unknown coefficients, or moments, are determined by substituting Eq. (2.8) into the Enskog equation and truncating consistently to order ε^k. Explicitly, this gives a set of equations for the (space- and time-dependent) coefficients:

$$\frac{\partial \rho A_{[n]}}{\partial t}\left\langle P_{[l]}(\vec{c}_1)\frac{1}{n!}P_{[n]}(\vec{c}_1)\right\rangle_0$$
$$+\frac{1}{2}\rho A_{[n]}\frac{\partial \ln T}{\partial t}\left\langle\left(\vec{c}\cdot\frac{\partial}{\partial \vec{c}_1}P_{[l]}(\vec{c}_1)\right)\frac{1}{n!}P_{[n]}(\vec{c}_1)\right\rangle_0$$
$$+\rho A_{[n]}\frac{\partial \vec{u}}{\partial t}\cdot\left\langle\left(\frac{\partial}{\partial \vec{c}_1}P_{[l]}(\vec{c}_1)\right)\frac{1}{n!}P_{[n]}(\vec{c}_1)\right\rangle_0$$
$$+\frac{\partial \rho A_{[n]}}{\partial \vec{q}}\cdot\left\langle \vec{v}P_{[l]}(\vec{c}_1)\frac{1}{n!}P_{[n]}(\vec{c}_1)\right\rangle_0$$
$$+\frac{1}{2}\rho A_{[n]}\frac{\partial \ln T}{\partial \vec{q}}\cdot\left\langle \vec{v}\left(\vec{c}\cdot\frac{\partial}{\partial \vec{c}_1}P_{[l]}(\vec{c}_1)\right)\frac{1}{n!}P_{[n]}(\vec{c}_1)\right\rangle_0$$
$$+\rho A_{[n]}\frac{\partial u_j}{\partial q_i}\left\langle v_i\left(\frac{\partial}{\partial c_{1j}}P_{[l]}(\vec{c}_1)\right)\frac{1}{n!}P_{[n]}(\vec{c}_1)\right\rangle_0$$
$$=\chi\int d\vec{v}_1 P_{[l]}(\vec{c}_1)J\left[\rho\phi\frac{1}{m!}A_{[m]}P_{[m]},\rho\phi\frac{1}{n!}A_{[n]}P_{[n]}\right], \tag{2.9}$$

where $\langle\ \rangle_0$ indicates a velocity average over the local-equilibrium ensemble and the factors of ε have been suppressed. Indeed, we can now set $\varepsilon=1$ since these equations, which can be viewed as an extension of the Navier-Stokes equations, are to be solved exactly. However, there are in general an infinite number of equations so that, as a final approximation, all but the first k equations are discarded (this is equivalent to projecting the Enskog equation onto the subspace spanned by the first k basis functions). For USF the moment equations reduce to

$$\frac{\partial A_{[l]}}{\partial t}\langle P_{[l]}(\vec{c}_1)P_{[n]}(\vec{c}_1)\rangle_0 + \frac{1}{2}A_{[n]}\frac{\partial \ln T}{\partial t}\left\langle \left(\vec{c}\cdot\frac{\partial}{\partial \vec{c}_1}P_{[l]}(\vec{c}_1)\right)P_{[n]}(\vec{c}_1)\right\rangle_0 + A_{[n]}a_{ji}\left\langle v_i\left(\frac{\partial}{\partial c_{1j}}P_{[l]}(\vec{c}_1)\right)P_{[n]}(\vec{c}_1)\right\rangle_0 + A_{[n]}\left\langle \left(\vec{c}\cdot\frac{\partial}{\partial \vec{c}_1}P_{[l]}(\vec{c}_1)\right)\vec{F}_{ext}P_{[n]}(\vec{c}_1)\right\rangle_0 = A_{[m]}A_{[n]}\rho\chi\int d\vec{v}_1 P_{[l]}(\vec{c}_1)J[\phi P_{[m]},\phi P_{[n]}]. \quad (2.10)$$

For USF, one expects that the distribution function is a continuous function of the velocity, so it is convenient to choose the basis functions to be the three-dimensional Hermite polynomials [20], which form a complete set and are mutually orthogonal. They are defined as

$$H_{i_1\cdots i_n}(\vec{p})\equiv n!(-1)^n e^{p^2/2}\frac{\partial}{\partial p_{i_1}}\cdots\frac{\partial}{\partial p_{i_n}}e^{-p^2/2} \quad (2.11)$$

and satisfy the orthogonality property

$$\left(\frac{1}{2\pi}\right)^{3/2}\int d\vec{p}e^{-p^2/2}H_{[n]}(\vec{p})H_{[m]}(\vec{p})=n!\,\delta_{nm}\delta_{[n][m]}, \quad (2.12)$$

with the multi-index Kronecker delta function defined as 0 if $n\neq m$ and

$$\delta_{[n][n']}\equiv\frac{1}{n!}\sum_{P\{i_1\cdots i_n\}}\delta_{i_1 i_1'}\cdots\delta_{i_n i_n'} \quad (2.13)$$

where the notation indicates that the sum is over all permutations of the indices. Two useful properties of the polynomials are

$$p_i H_{j_1\cdots j_n}(\vec{p})=H_{ij_1\cdots j_n}(\vec{p})+n\delta_{i(j_1}H_{j_2\cdots j_n)}(\vec{p}),$$
$$\frac{\partial}{\partial p_i}H_{j_1\cdots j_n}(\vec{p})=n\delta_{i(j_1}H_{j_2\cdots j_n)}(\vec{p}), \quad (2.14)$$

where we use a special notation in which symmetrized indices are grouped by round parenthesis (e.g., $\delta_{(ij)}\equiv\frac{1}{2!}(\delta_{ij}+\delta_{ji})$. In this case, it follows that $\langle H_{[n]}(\vec{c})\rangle=A_{[n]}$ and, in particular, $\langle\frac{1}{2}v'^2\rangle=\frac{1}{2}k_BT\langle H_{rr}(\vec{c})+3H_{[0]}\rangle=\frac{3}{2}k_BT+\frac{1}{2}k_BTA_{rr}$ so that, in general, one must impose the conditions $A_{[0]}=A_{[1]}=A_{rr}=0$. Consequently, the density, velocity and energy fields are, in the general case, determined by the conservation equations (2.5), while the other moments are determined from Eq. (2.9). An alternative choice of basis that is closely related to the more familiar Chapman-Enskog expansion is to take the set $\{P_{[n]}(\vec{p})\}$ to be the traceless, symmetric tensors of order n [20]. These are simply related to the spherical harmonics [20] and represent an expansion in the angular dependence of the distribution. This set is particularly useful for generating an expansion in the gradients of the hydrodynamic fields since their tracelessness means that the coefficients of the expansion can only be constructed from the gradients: Terms involving unit tensors give no contribution. Thus, for USF, a solution to second order in the shear rate only requires the retention of terms in the series to fourth order in the momentum. However, although polynomials of different order are orthogonal under an angular integration, they do not form a complete set and the coefficients of the expansion depend in general on the magnitude of the momentum. Practically, this necessitates a second expansion of this scalar dependence for which the Sonine polynomials are usually used (the so-called Chapman-Cowling expansion [2,3]). In fact, for the case of a steady state in which only a single gradient is present, as in USF, the Chapman-Enskog expansion is essentially a moment expansion ordered by the gradient, although it is not usually phrased as such. In summary, let us note that these different possibilities are all equivalent, differing only in the particular terms included or excluded at a given order in the expansions: a difference that should be of minor importance if the expansions are to be useful.

For USF, the tensorial nature of the coefficients must derive from the shear tensor and the unit tensor, which immediately implies that only even terms can occur in the expansion. The moment equations reduce to

$$n(a\delta_{rx}\delta_{sy}+\gamma\delta_{rs})[\varepsilon^n\delta_{r(i_1}A_{i_2\cdots i_n)s}+(n-1)\varepsilon^{n-2}\delta_{r(i_1}A_{i_2\cdots i_{n-1}}\delta_{i_n)s} = D_{[i_1\cdots i_n]}+\varepsilon^l C_{[i_1\cdots i_n][l]}A_{[l]} + \varepsilon^{l+m}B_{[i_1\cdots i_n][l][m]}A_{[l]}A_{[m]}, \quad (2.15)$$

with

$$B_{[i_1\cdots i_n][l][m]} \equiv \rho\chi\frac{1}{l!m!}\int d\vec{v}_1 H_{[i_1\cdots i_n]}(\vec{c}_1)J[\phi H_{[l]},\phi H_{[m]}],$$
$$C_{[i_1\cdots i_n][l]}=B_{[i_1\cdots i_n][0][l]}+B_{[i_1\cdots i_n][l][0]},$$
$$D_{[i_1\cdots i_n]}=B_{[i_1\cdots i_n][0][0]}, \quad (2.16)$$

and the condition $A_{rr}=0$ serves to define the thermostat constant. These equations exhibit an important feature of USF, which is the fact that the kinematic terms, on the left-hand side of Eq. (2.15), only couple the nth equation to moments of order n and lower (specifically, only n and $n-2$). In the case of Maxwell molecules, the forward couplings, i.e., couplings of the nth equation to moments of order $n+1$ or higher, which occur on the right-hand side of the equations, are exactly zero, which is the reason the system can be solved [20]. As shown below, the forward couplings have a relatively small effect in the present case, thus giving some heuristic justification for the moment method.

Summarizing, the approximation to the kinetic equation is obtained by neglecting all terms in Eqs. (2.8) and (2.15) above order ε^k. There are still an infinite number of equations and now only a finite number of coefficients to determine, so it is necessary to introduce a further approximation according to which we neglect all but the first k equations. Effectively, this corresponds to projecting the Enskog equation into the subspace spanned by the first k basis functions. As the order of the approximation increases, this procedure generates a sequence of approximations to the full kinetic equation. To order ε^4, one finds

$$\begin{aligned}
&2(a\delta_{xr}\delta_{ys}+\gamma\delta_{rs})(\delta_{r(i}\delta_{j)s}+\delta_{r(i}A_{j)s}\\
&\quad=(D_{ij}+C_{[ij][2']}A_{[2']}+C_{[ij][4']}A_{[4']}\\
&\qquad+B_{[ij][2'][2'']}A_{[2']}A_{[2'']}),\\
&4(a\delta_{xr}\delta_{ys}+\gamma\delta_{rs})(\delta_{r(i}A_{jlm)s}+3\delta_{r(i}A_{jl}\delta_{ms)}\\
&\quad=(D_{ijlm}+C_{ijlm,[2']}A_{[2']}+C_{ijlm,[4']}A_{[4']}\\
&\qquad+B_{ijlm,[2'][2'']}A_{[2']}A_{[2'']}),
\end{aligned}\tag{2.17}$$

together with the equation fixing the thermostat

$$\begin{aligned}
2aA_{xy}+6\gamma=(&D_{rr}+C_{[rr][2']}A_{[2']}+C_{[rr][4']}A_{[4']}\\
&+B_{[rr][2'][2'']}A_{[2']}A_{[2'']}).
\end{aligned}\tag{2.18}$$

The primary difference between the solution of the Boltzmann equation and the Enskog equation for USF is that for the Boltzmann equation, the coefficients appearing on the right-hand sides of these equations are shear-rate independent, whereas for the Enskog equation, they have a complex dependence on the shear rate.

A. Perturbative solution

The evaluation and expansion of the coefficients appearing in Eq. (2.17) is discussed in the appendixes. It is also necessary to expand the coefficients $A_{[2]}$ and $A_{[4]}$ in the shear rate as, e.g., $A_{i_1i_2}=aA^{(1)}_{i_1i_2}+a^2A^{(2)}_{i_1i_2}+\cdots$. Since the only two tensors available are the shear tensor and the unit tensor, the coefficients to first order in the shear rate must have the form $A^{(1)}_{i_1\cdots i_n}=n!\,\nu_n\delta_{x(i_1}\cdots\delta_{i_n)y}$, where ν_n is to be determined. Similarly, the second-order contributions must have the form

$$A^{(2)}_{ij}=2(\varepsilon_1\delta_{ij}+\varepsilon_2\delta_{x(i}\delta_{j)x}+\varepsilon_3\delta_{y(i}\delta_{j)y},\tag{2.19}$$

$$\begin{aligned}
A^{(2)}_{ijlm}=24(&\sigma_1\delta_{(ij}\delta_{lm)}+\sigma_2\delta_{x(i}\delta_{jl}\delta_{mx)}+\sigma_3\delta_{y(i}\delta_{jl}\delta_{m)y}\\
&+\sigma_4\delta_{(xxyy)(ijlm)}),
\end{aligned}$$

with the condition that $3\varepsilon_1+\varepsilon_2+\varepsilon_3=0$. Straightforward calculation then leads to a set of linear equations for the coefficients (details are given in Appendix B). The first-order coefficients are found to be

$$\nu_2=\left(\frac{205}{202}\right)\mu,\quad \nu_4=-\frac{6}{205}\nu_2,\tag{2.20}$$

with

$$\mu=-\left[\frac{5}{16\rho\chi\sqrt{\pi}}\left(1+\frac{4\pi}{15}\rho\chi\right)\right],$$

while the second-order coefficients are

$$\begin{aligned}
\varepsilon_2&=\varepsilon_3-\frac{1025}{3232\rho\chi\sqrt{\pi}}\nu_2+\frac{105}{808\rho\chi\sqrt{\pi}}\nu_4,\\
\varepsilon_3&=\frac{199}{8484}+\frac{15}{808\rho\chi\sqrt{\pi}}\left(1+\frac{47}{63}\rho\chi\pi\right)\nu_2-\frac{5}{202}\nu_2^2\\
&\quad+\frac{5}{707}\sqrt{\pi}\nu_4,\\
\sigma_1&=\gamma_1-\frac{1}{3}\gamma_2-\frac{1}{3}\gamma_3+\frac{1}{35}\gamma_4,\\
\sigma_2&=\gamma_2-\frac{1}{7}\gamma_4,\\
\sigma_3&=\gamma_3-\frac{1}{7}\gamma_4,\\
\sigma_4&=\gamma_4,
\end{aligned}\tag{2.21}$$

with

$$\begin{aligned}
\gamma_1&=\frac{1}{480}-\frac{1}{32\rho\chi\sqrt{\pi}}\left(1+\frac{4}{15}\rho\chi\pi\right)\nu_2-\frac{1}{60}\nu_2^2\\
&\quad-\frac{5}{32\rho\chi\sqrt{\pi}}\left(1+\frac{22}{75}\rho\chi\pi\right)\nu_4,\\
\gamma_2&=\gamma_3+\frac{15}{1616\rho\chi\sqrt{\pi}}\nu_2-\frac{105}{404\rho\chi\sqrt{\pi}}\nu_4,\\
\gamma_3&=\frac{1}{1414}-\frac{15}{404\rho\chi\sqrt{\pi}}\left(1+\frac{11}{105}\rho\chi\pi\right)\nu_2-\frac{31}{1414}\nu_2^2\\
&\quad-\frac{10}{707}\sqrt{\pi}\nu_4,\\
\gamma_4&=\frac{1}{687}-\frac{315}{1832\rho\chi\sqrt{\pi}}\left(1+\frac{44}{315}\rho\chi\pi\right)\nu_2+\frac{23}{458}\nu_2^2\\
&\quad-\frac{23}{458}\sqrt{\pi}\nu_4.
\end{aligned}\tag{2.22}$$

The exact value [2] of ν_2 is 1.016μ compared to the present result of $\frac{205}{202}\mu=1.015\mu$. It is interesting to compare these results with those obtained if the forward couplings in the moment equations are neglected. In this case, $\nu_2=\mu$, $\nu_4=0$, and

$$\begin{aligned}
\varepsilon_2&=\varepsilon_3-\frac{5}{16\sqrt{\pi}\rho\chi}\nu_2,\\
\varepsilon_3&=\frac{1}{42}+\frac{1}{84}\sqrt{\pi}\nu_2-\frac{1}{28}\nu_2^2.
\end{aligned}\tag{2.23}$$

By way of comparison, if taking $\rho\chi=1$ (i.e., ρ slightly less than 0.5), then the full solution gives $\nu_2=-0.3288$,

$\nu_4=0.0096$, $\varepsilon_2-\varepsilon_3=0.0595$, and $\varepsilon_3=0.0094$, whereas without the forward couplings the result is $\nu_2=-0.3240$, $\nu_4=0.0$, $\varepsilon_2-\varepsilon_3=0.0571$, and $\varepsilon_3=0.0132$. Although not completely negligible, the effect of the forward couplings are nevertheless relatively small, being comparable to the difference between the exact value of ν_2 and the simplest approximation $\nu_2=\mu$.

Combining Eqs. (2.19) and (2.8) gives the explicit form of the distribution to fourth order in the moments and to second order in the shear rate:

$$\begin{aligned}f(\vec{p})=\rho\phi(\vec{p})\{&1+a[\nu_2+\nu_4(p^2-7)]p_xp_y+a^2\gamma_1(p^4-10p^2\\&+15)+a^2[\varepsilon_2+\gamma_2(p^2-7)](p_x^2-\tfrac{1}{3}p^2)\\&+a^2[\varepsilon_3+\gamma_3(p^2-7)](p_y^2-\tfrac{1}{3}p^2\}\\&+a^2\gamma_4(p_x^2p_y^2-\tfrac{1}{7}p^2p_x^2-\tfrac{1}{7}p^2p_y^2+\tfrac{1}{35}p^4)\}+o(a)^3.\end{aligned} \tag{2.24}$$

The pressure tensor for a homogeneous system is given by

$$P_{ij}=\rho A_{ij}+\frac{1}{2}m\sigma^3\chi\left\langle\int d\hat{q}\ \Theta(\hat{q}\cdot\vec{g})(\hat{q}\cdot\vec{g})^2\hat{q}_i\hat{q}_j\right\rangle \tag{2.25}$$

where the integral is over the unit sphere. Straightforward calculation gives for the pressure

$$P-p_0=2a^2\rho\left[\frac{\sqrt{\pi}}{105}\chi\rho\left(\frac{1}{2}\sqrt{\pi}-2\nu_2+\nu_4\right)\right]+o(a^3), \tag{2.26}$$

where the equilibrium pressure is $p_0=\rho[1+(2\pi/3)\rho\chi]$. The normal stresses are

$$\begin{aligned}P_{xx}-P_{yy}&=2a^2\rho(\varepsilon_2-\varepsilon_3)\left(1+\frac{4\pi}{15}\rho\chi\right)+o(a^3),\\P_{xx}-P_{zz}&=2a^2\rho\left[\varepsilon_2\left(1+\frac{4\pi}{15}\rho\chi\right)\right.\\&\quad\left.+\frac{2\sqrt{\pi}}{45}\rho\chi\left(\frac{1}{2}\sqrt{\pi}+2\nu_2+\nu_4\right)\right]+o(a^3)\end{aligned} \tag{2.27}$$

and the only off-diagonal component is

$$P_{xy}=P_{yx}=-\rho a\left[\nu_2\left(1+\frac{4\pi}{15}\rho\chi\right)+\frac{4\sqrt{\pi}}{15}\rho\chi\right]+(a^3). \tag{2.28}$$

These expressions may all be decomposed into the sum of a kinetic contribution (zeroth order in $\rho\chi$) and a collisional contribution (first order in $\rho\chi$). The accuracy of Eqs. (2.26) and (2.27) has recently been confirmed by comparison to direct simulation of the Enskog equation [26].

B. Nonperturbative solution

The validity of the perturbative solution is obviously restricted to the case of small gradients. It is not clear, however, that the approximate moment equations are so constrained. In the case of Maxwell molecules, the forward couplings vanish identically irrespective of the size of the gradients and, as we have seen, their neglect has relatively little effect on the perturbative results. It therefore seems reasonable to solve these equations without the assumption of small gradients. Because of the difficulty of carrying out the calculations, only the equations for the second moments

$$\begin{aligned}2a(\delta_{x(i}\delta_{j)y}+\delta_{x(i}A_{j)y})+2\gamma(\delta_{ij}+A_{ij})\\=C_{ij[0]}+C_{ij,lm}A_{lm},\end{aligned} \tag{2.29}$$

$$2aA_{xy}+6\gamma=C_{rr[0]}+C_{rr,lm}A_{lm}, \tag{2.30}$$

with the (exact) coefficients

$$\begin{aligned}C_{ij[0]}=\rho\chi\int d\hat{q}q_iq_j\left\{\frac{1}{\sqrt{\pi}}w^2e^{-w^2/4}+\frac{1}{2}w(w^2+2)\right.\\\left.\times\left[\operatorname{erf}\left(\frac{1}{2}w\right)-1\right]\right\},\end{aligned} \tag{2.31}$$

$$\begin{aligned}C_{ij,lm}=\frac{1}{2}\rho\chi\int d\hat{q}\Bigg(&\left\{\frac{8}{\sqrt{\pi}}e^{-w^2/4}+6w\left[\operatorname{erf}\left(\frac{1}{2}w\right)-1\right]\right.\\&\times q_iq_jq_lq_m-\left\{\frac{2}{\sqrt{\pi}}e^{-w^2/4}+w\left[\operatorname{erf}\left(\frac{1}{2}w\right)-1\right]\right\}\\&\times(q_jq_l\delta_{im}+q_jq_m\delta_{il}+q_iq_l\delta_{jm}+q_iq_m\delta_{jl})\\&-\left\{\frac{2}{3\sqrt{\pi}}(w^2+8)e^{-w^2/4}\right.\\&\left.+\frac{1}{3}w(10+w^2)\left[\operatorname{erf}\left(\frac{1}{2}w\right)-1\right]\right\}q_iq_j\delta_{lm}\Bigg).\end{aligned}$$

are considered here. These are solved numerically using a quasi-Newton method [27]. Numerically, better convergence is achieved by replacing Eq. (2.30) by the original condition $A_{xx}+A_{yy}+A_{zz}=0$. All of the calculations presented below are accurate to one part in 10^4 or better.

III. COMPARISON TO MOLECULAR DYNAMICS

In order to evaluate these results, I have performed nonequilibrium molecular dynamics (MD) simulations of a hard-sphere fluid with density $\rho\sigma^3=0.5$ (about one-half the freezing density and sufficiently high that collisional effects are important). The flow state is imposed by means of Lees-Edwards boundary conditions and the temperature is maintained approximately constant at a value $k_BT_0=1$ by rescaling the velocities to give a temperature of $0.95T_0$ whenever the temperature exceeds $1.05T_0$. For each value of the shear rate, the simulations begin with an equilibrated fluid and are run for 3×10^6 collisions to reach the steady state. The systems are then run an addtional 3×10^6collisions to accumulate the statistics. The various quantities are average for 10 000 collisions and recorded. The errors are estimated using Erpenbeck's pooling method [28], according to which

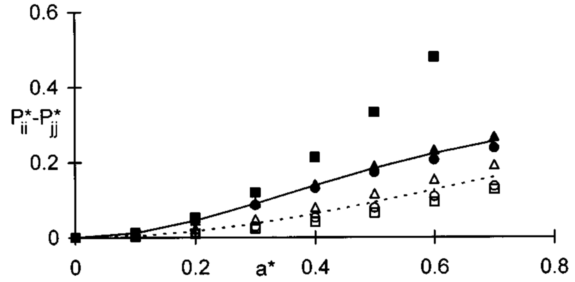

FIG. 1. Kinetic parts of the reduced normal stresses $P^*_{xx}-P^*_{yy}$, where the dimensionless pressure tensor is $P^*_{ij}=P_{ij}/\rho k_BT$, as a function of reduced shear rate ($a^*=a/4\rho\sqrt{\pi k_BT}$) for $\rho=0.5$ as determined from simulation (filled circles), the perturbative calculation (filled squares), the nonperturbative calculation (solid line), and the proposed kinetic model [Eq. (4.8)] (filled triangles). The corresponding results for $P^*_{yy}-P^*_{zz}$ are shown with open symbols.

the recorded values are averaged, or pooled, over some fixed period, say, in groups of 50 000 collisions. The standard error (standard deviation divided by the square root of the number of samples) is then computed over these pooled values. These estimated errors are found to be insensitive to the exact choice for the period and are in all cases comparable to or smaller than the size of the symbols used in the figures below.

Figure 1 shows a comparison of the kinetic parts of the normal stresses as calculated from the two analytic solutions and the MD results. The simulations span a range of shear rates from equilibrium to $a^*=a/4\rho\sqrt{\pi k_BT}=0.7$: Above this the fluid begins to order and the present analysis becomes inapplicable [29]. The value of χ has been taken to give the equilibrium pressure as determined in the simulations. Note that because of the thermostat, the kinetic contribution to the pressure is fixed so there are only two independent normal stresses. Both calculations give good approximations for $P_{yy}-P_{zz}$, with the perturbative calculation being slightly better. However, for $P_{xx}-P_{yy}$ the perturbative estimate is only accurate for small shear rates whereas the nonperturbative estimate is in reasonable agreement over the entire range of shear rates. The reason for this can be seen in Fig. 2, which shows the same data in the form of the viscometric functions defined as $\psi_1=(P_{xx}-P_{yy})/a^2$ and $\psi_2=(P_{yy}-P_{zz})/a^2$. The latter is nearly constant over the entire range of shear rates so that the inclusion of the fourth-order moments in the perturbative calculation improves the agreement relative to the nonperturbative estimate. In contrast, the first viscometric function exhibits a strong shear-rate dependence so that only its asymptotic value is estimated in the perturbative calculation. Another qualitative difference between the two approximations is that the nonperturbative solution gives a semiquantitative model for shear thinning whereas this is absent from the perturbative solution since it is an order a^3 effect. Figure 3 compares the kinetic contributions to the shear viscosity defined as $\eta=-P_{xy}/a$. The agreement is reasonable over the entire range of shear rates with the model accounting for about 80% of the decrease of the viscosity at $a^*=0.7$.

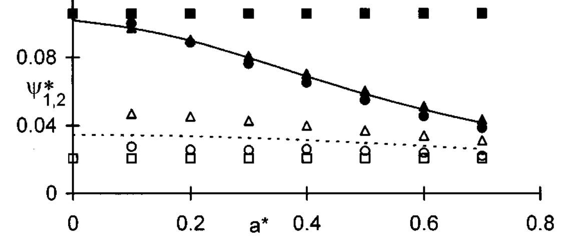

FIG. 2. Kinetic parts of the reduced viscometric functions for $\rho=0.5$ (same legend as Fig. 1).

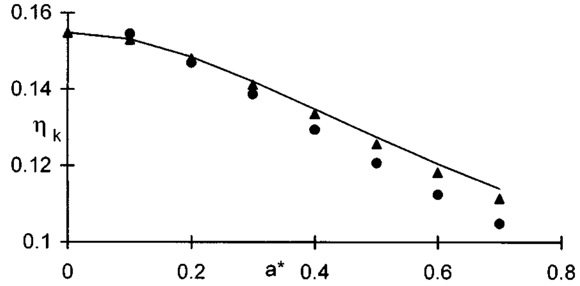

FIG. 3. Kinetic part of the shear viscosity as a function of reduced shear rate for $\rho=0.5$. The circles are from MD, the line is calculated from the nonperturbative theory, and the triangles are from the proposed kinetic theory.

The collisional contributions to the pressure tensor involve an additional approximation compared to the kinetic parts since they depend in general on all of the moments. Thus one does not expect the results of either of the calculations to be as accurate at large shear rates as in the case of the kinetic parts. The collisional contributions to the normal stresses are compared in Fig. 4 and, as expected, the agreement is poorer than for the kinetic contributions. Somewhat surprisingly, the collisional contributions to the pressure (Fig. 5) are extremely well modeled by the nonperturbative calculation. The worst agreement is in the collisional contributions to the shear viscosity as shown in Fig. 6. Although the effects are very small, it is nevertheless the case that the calculated decrease up to $a^*=0.7$ is only about a one-third of the actual decrease, which seems to indicate that it is the most sensitive to the truncation of the expansion of the collision integrals.

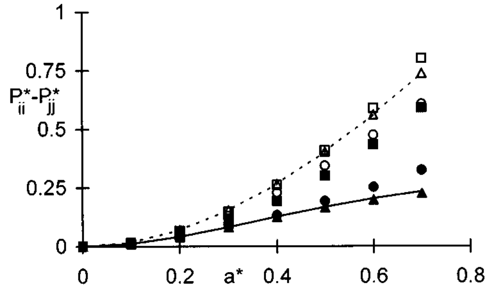

FIG. 4. Collisional parts of the reduced normal stresses for $\rho=0.5$ (same legend as Fig. 1, except that now the triangles are the maximum entropy result [Eq. (4.15)].

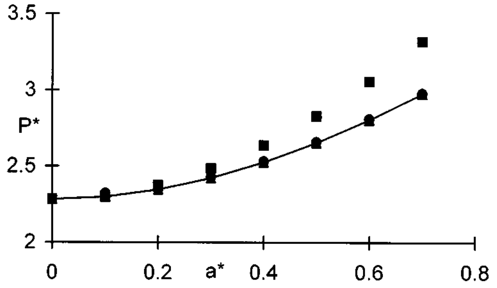

FIG. 5. Collisional contribution to the reduced pressure as a function of reduced shear rate for $\rho=0.5$ (same legend as Fig. 4).

IV. CONCLUSIONS

The calculations presented here serve to show that the Enskog equation can be used to describe nonequilibrium fluid properties at moderate density extend well beyond the linear regime. The perturbative calculations are in good agreement with the simulations at small shear rates and only for particular properties differ significantly at large shear rates. The nonperturbative calculations illustrate an alternative means of analyzing the Enskog equation and yield, with relatively little effort, a more realistic description of the normal stresses and a semiquantitative model of shear thinning at large shear rates. It is clear that low-order moment expansions of the distribution are of limited use in describing collisional transfer even when they are accurately determined.

These results are also of some relevance to a recent attempt to formulate a kinetic model of the Enskog equation. The simplest kinetic model of the Boltzmann equation is the Bhatner-Gross-Kook (BGK) model, which is based on the observation that the Boltzmann collision operator can be written in the form

$$J[f,f]=-\nu\{f(1)-\phi(1)\} \tag{4.1}$$

(see Appendix A) where, in the BGK approximation, the velocity-dependent prefactor is approximated by a (constant) relaxation time and the second term in square brackets by the local equilibrium (LE) distribution function. These approximations are based on the fact that the LE distribution is in the null space of the Boltzmann operator and on the idea that the main role of collisions is to drive the system towards (local) equilibrium. For USF, the BGK equation becomes

$$-av_y\frac{\partial}{\partial v_x}f+\gamma\frac{\partial}{\partial \vec{v}}\cdot\vec{v}f=-\nu(f-\phi). \tag{4.2}$$

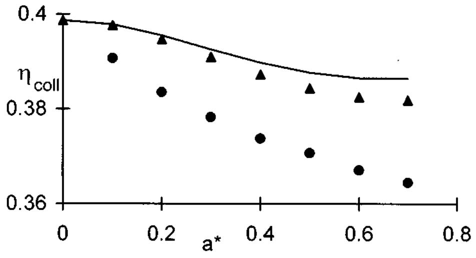

FIG. 6. Collisional contribution to the shear viscosity for $\rho=0.5$. The circles are from MD, the line is from the nonperturbative theory, and the triangles are the maximum entropy result [Eq. (4.15)].

The extension of this model to the Enskog equation is not straightforward. In part, this is due to the fact that the LE distribution is not in the null eigenspace of the Enskog operator. An obvious remedy is to write

$$J[f,f]=J[\phi,\phi]+(J[f,f]-J[\phi,\phi])\approx J[\phi,\phi]-\nu(f-\phi), \tag{4.3}$$

which reduces to the BGK model for the Boltzmann operator while giving a part of the collisional transfer that distinguishes the Enskog operator. However, the equation for the thermostat that results is

$$-\langle av_yv_x\rangle-3(\rho k_BT)\gamma=\rho\chi\int d\vec{v}\; v^2J[\phi,\phi], \tag{4.4}$$

which differs from the Enskog result (2.7) in that the collisional term on the right-hand side is evaluated using the LE distribution so that only a part of the collisional contribution to the viscosity is obtained. This suggests that more careful treatment of the collisional term is needed. To this end, note that, in terms of the moment equations, the original BGK approximation replaces all of the collisional coefficients by a single representative eigenvalue [21] $B^{BGK}_{[n][l][m]}=-\nu(\delta_{l0}\delta_{[n][m]}+\delta_{m0}\delta_{[n][l]})$. The approximation suggested above [Eq. (4.3)], for the Enskog operator keeps all moments of the LE term but replaces all others by an eigenvalue. In particular, this means that the coefficients $B_{[n][0][0]}$ are retained exactly and the others approximated: The obvious extension is to retain more of the moments. This suggests a class of approximations whereby the collision operator is separated into two pieces as above, in which the local-equilibrium term is kept exactly as is some subset of the moments of the second piece. The higher moments are treated approximated with a single relaxation time giving the general approximation

$$\begin{aligned}J[f,f]&=\sum_{n,l,m}H_{[n]}B_{[n][l][m]}A_{[l]}A_{[m]}\\&\simeq\sum_{n}H_{[n]}B_{[n][0][0]}+\sum_{\substack{n,l,m\in S\\ l+m>0}}H_{[n]}B_{[n][l][m]}A_{[l]}A_{[m]}\\&\quad+\sum_{\substack{n,l,m\notin S\\ l+m>0}}H_{[n]}B^{BGK}_{[n][l][m]}A_{[l]}A_{[m]}\\&=J[\phi,\phi]+\sum_{\substack{n,l,m\in S\\ l+m>0}}H_{[n]}B_{[n][l][m]}A_{[l]}A_{[m]}\\&\quad-\nu\Bigg(f-\phi-\sum_{\substack{n\in S\\ n>0}}H_{[n]}A_{[n]}\Bigg),\end{aligned} \tag{4.5}$$

where the set of moments retained exactly is indicated by the notation $n,l,m\in S$ (this notation is schematic and, in particular, does not imply that the *same* terms be used in the sum over n as in that over l,m). This must be supplemented by the self-consistency condition

$$A_{[l]}=\langle H_{[l]}\rangle \tag{4.6}$$

for all l. Except for the special treatment of the local-equilibrium term, this is a direct generalization of the Gross-Jackson extension [30,21] of the BGK model. Notice that this involves two types of approximation. The first is the choice of moments $A_{[l]}$ retained in the first sum on the third line that arise from approximating the distribution by its moment expansion. The second approximation is the selection of the number of terms retained in the expansion of the collision operator itself (i.e., the range of the sums over n). Before discussing specific choices, we note that one deficiency of this model is that it does not reduce to the standard BGK model at low density. To achieve this correspondence, one should separate out the Boltzmann contributions by writing

$$\begin{aligned}J[f,f]\simeq{}&J[\phi,\phi]+\sum_{\substack{n,l,m\in S\\ l+m>0}}H_{[n]}B_{[n][l][m]}A_{[l]}A_{[m]}\\&-\nu\left(f-\phi-\sum_{n>0;n\in S}H_{[n]}A_{[m]}\right)\\={}&J[\phi,\phi]+\sum_{\substack{n,l,m\in S\\ l+m>0}}H_{[n]}(B_{[n][l][m]}-B^{B}_{[n][l][m]})\\&\times A_{[l]}A_{[m]}-\nu(f-\phi)\\&+\sum_{\substack{n,l,m\in S\\ l+m>0}}H_{[n]}(B^{B}_{[n][l][m]}-B^{BGK}_{[n][l][m]})A_{[l]}A_{[m]},\end{aligned} \tag{4.7}$$

where $B^{B}_{[n][l][m]}$ are the couplings in the Boltzmann limit. Neglect of the last term is part of the BGK approximation to the Boltzmann equation and so it is consistent to drop it, giving the general BGK-like approximation to the Enskog equation

$$\begin{aligned}\frac{\partial}{\partial t}f+\vec{v}\cdot\frac{\partial}{\partial\vec{q}}f+\frac{\partial}{\partial\vec{v}}\cdot\vec{F}_{ext}f={}&J[\phi,\phi]-\nu(f-\phi)\\&+\sum_{\substack{n,l,m\in S\\ l+m>0}}H_{[n]}(B_{[n][l][m]}\\&-B^{B}_{[n][l][m]})A_{[l]}A_{[m]}\end{aligned} \tag{4.8}$$

together with the self-consistency relation (4.6). The price paid for maintaining contact with the usual BGK approximation is that while Eq. (4.5) can be systematically extended, by the inclusion of more moments, to (presumably) approximate the Enskog equation arbitrarily closely, Eq. (4.8) can only be a model of the Enskog equation since it rests on an uncontrolled approximation.

The kinetic model for the Enskog equation suggested in Ref. [11], henceforth referred to as the Dufty-Santos-Brey (DSB) model, consists of taking all values of l,m above and restricting the sum over n to include only the projections onto $\{H_{[0]}=1,H_{[1]}=\vec{c},H_{[rr]}=c^2-3\}$. [To project onto H_{rr} one writes $H_{ij}=\frac{1}{3}H_{rr}\delta_{ij}+(H_{ij}-\frac{1}{3}H_{rr}\delta_{ij})$ and ignores the contributions from the second (traceless) term.] Additionally, the DSB model also expands the term $J[\phi,\phi]$ in Hermite polynomials and makes the same truncation of the series, but this difference is not of conceptual importance, although it does lead to quantitatively inaccurate transport coefficients. It is instructive to consider the moment equations obtained in this approximation for the case of USF:

$$\begin{aligned}&(a\,\delta_{rx}\delta_{sy}+\gamma\delta_{rs})(n\,\delta_{r(i_1}A_{i_2\cdots i_n)s}+\delta_{r(i_1}A_{i_2\cdots i_{n-1}}\delta_{i_n)s})\\&\quad=D_{i_1\cdots i_n}-\nu A_{i_1\cdots i_n}+\delta_{n2}\delta_{ij}\sum_{l+m>0}(B_{[rr][l][m]}\\&\qquad-B^{B}_{[rr][l][m]})A_{[l]}A_{[m]}.\end{aligned} \tag{4.9}$$

The main simplifying feature of this model is the decoupling of the moments for $n>2$. For example, the equations for the fourth moments are

$$\begin{aligned}&(a\,\delta_{rx}\delta_{sy}+\gamma\delta_{rs})(n\,\delta_{r(i}A_{jlm)s}+\delta_{r(i}A_{jl}\delta_{m)s}\\&\quad=D_{ijlm}-\nu A_{ijlm},\end{aligned} \tag{4.10}$$

so that it is possible to immediately solve for the fourth moment (or in general all moments for $n>2$) in terms of the second moments which are determined by the nonlinear equation (4.9). However, to carry through this program still requires the evaluation of the entire (infinite) set of couplings entering into Eq. (4.9), which is, of course, impractical. In fact, for USF the model is not actually any easier to solve than is the model obtained by retaining the full set of moment equations and dropping the forward couplings (which has the advantage of being the first step in a systematic solution of the Enskog equation). On the other hand, the DSB model does have the key simplifying feature of the BGK and Jackson-Gross models which is that the velocity dependence of the distribution is simple and explicitly given [21]. An obvious simplification is to limit the moments entering into the DSB model, namely, A_{lm} and A_{lmr}. The simplicity of the BGK model is only achieved by limiting attention to the linear terms giving a very simple model

$$\begin{aligned}&\frac{\partial}{\partial t}f+\vec{v}\cdot\frac{\partial}{\partial\vec{q}}f+\frac{\partial}{\partial\vec{v}}\cdot\vec{F}_{ext}f\\&\quad=J[\phi,\phi]-\nu(f-\phi)+c_i\Delta C_{i,lm}A_{lm}\\&\qquad+(c^2-3)\frac{1}{3}(\Delta C_{ss,lm}A_{lm}+\Delta C_{ss,lmr}A_{lmr}),\end{aligned} \tag{4.11}$$

where $\Delta C_{rr,lm}=C_{rr,lm}-C^{B}_{rr,lm}$ and which, with the self-consistency condition (4.6), gives a simpler and more quantitatively accurate kinetic model than the original DSB proposal. For USF this becomes

$$\begin{aligned}-ac_y\frac{\partial}{\partial c_x}f+\gamma\frac{\partial}{\partial\vec{c}}\cdot\vec{c}f={}&J[\phi,\phi]+\left(\frac{1}{3}c^2-1\right)\Delta C_{ss,lm}A_{lm}\\&-\nu[f(\vec{c})-\phi],\end{aligned} \tag{4.12}$$

from which the equation for the second moments are easily found to be

$$2(a\delta_{rx}\delta_{sy}+\gamma\delta_{rs})(\delta_{r(i)}A_{(j)s}+\delta_{r(i)}\delta_{(j)s})$$
$$=D_{ij}+\delta_{ij}\frac{1}{3}\Delta C_{rr,lm}A_{lm}-\nu A_{ij} \qquad (4.13)$$

together with the usual condition that $A_{rr}=0$. The coefficients $\Delta C_{rr,lm}=C_{rr,lm}-C^{B}_{rr,lm}=C_{rr,lm}(a)-C_{rr,lm}(0)$, where $C_{rr,lm}(a)$ is the same as in Eq. (2.33). After solving for A_{ij}, Eq. (4.11) can be directly integrated to give the full distribution. Choosing the relaxation time to give the correct viscosity in the low-density (Boltzmann) limit gives $\nu=16\sqrt{\pi}\rho\chi/5$. This model, based on the DSB proposal but extended by inclusion of the local-equilibrium $J[\phi,\phi]$ terms and simplified by keeping only the linear, second moment contributions, is in surprising agreement with both the nonperturbative results given above and the simulations. The equilibrium shear viscosity is

$$\eta=-\rho\left[\mu\left(1+\frac{4\pi}{15}\rho\chi\right)+\frac{4\sqrt{\pi}}{15}\rho\chi\right],$$

which is the usual (lowest Sonine) Enskog result. The kinetic parts of the viscometric functions as calculated with this model are shown in Figs. 1–3 and are seen to be comparable to the moment solution. For the shear viscosity, the decrease of the kinetic contribution with increasing shear rate is even somewhat closer to the simulation values than in the nonperturbative calculation.

Although these results show that it is possible to construct simple kinetic models of the Enskog equation, they are of limited value in the study of USF far from equilibrium beause even in this simple case, the analytic form of the distribution is sufficiently complicated that it is not possible to calculate collisional contributions, e.g., to the pressure tensor, analytically. Given the recent development of numerical methods of solving the Enskog equation itself, there seems to be little incentive to carry through the calculations for the kinetic model numerically. To develop a useful approximate distribution, it is interesting to consider a proposal of Ordóñez, Brey, and Santos [31] in the context of the Boltzmann equation which is that the nonequilibrium distribution be modeled by maximizing the entropy $-\int d\vec{q}\, d\vec{v}'f(\vec{q},\vec{v}')\ln f(\vec{q},\vec{v}')$, subject to the constraint that the known moments be reproduced [in the present case that $\langle H_{[n]}(\vec{c})\rangle=A_{[n]}$ for the known moments $A_{[n]}$]. Requiring agreement through the second moments gives

$$f(\vec{q},\vec{v})=\rho\left(\frac{1}{2\pi k_BT}\right)^{3/2}(\det\Delta)^{-1/2}\exp\left(-\frac{1}{2k_BT}\vec{v}\cdot\Delta^{-1}\cdot\vec{v}\right), \qquad (4.14)$$

with $\Delta_{ij}=\delta_{ij}+A_{ij}$. As an example of the use of this approximation, the kinetic contributions to the pressure are, by construction, the same as those obtained from the model used to evaluate the second moments, while the collisional contributions are easily determined to be

$$\frac{1}{\rho k_BT}P^{(c)}_{ij}=2\rho\chi\int d\hat{q}\;\hat{q}_i\hat{q}_j u^2F\left(\frac{w}{2u}\right), \qquad (4.15)$$

with

$$u=\sqrt{1+A_{ij}\hat{q}_i\hat{q}_j},$$
$$w=a\hat{q}_x\hat{q}_y \qquad (4.16)$$

$$F(x)=\frac{1+2x^2}{4}[1-\mathrm{erf}(x)]-\frac{x}{2\sqrt{\pi}}e^{-x^2}.$$

The results using this model, with the second moments taken from the nonperturbative calculation, are also shown in Figs. 4–6 and are seen to be comparable to, or even slightly better than, using the second moments. For kinetic theory calculations of the properties of strongly sheared fluids, such as those presented in Refs. [17,18,29], which are based on the first-order (in the shear) perturbative correction to the equilibrium distribution, the use of the model distribution given by Eqs. (4.15) and (4.16), which is simple, positive definite, and gives a qualitative description of nonlinear effects such as shear thinning and normal stresses, would appear to be a more realistic alternative and is currently being investigated.

In summary, these results show that the Enskog equation can be used to predict the properties of a sheared fluid well into the nonlinear regime by means of the moment expansion. It has been shown that this information can be used to extend and simplify the DSB model to give a simple kinetic model of the Enskog equation, which, like the BGK model on which it is based, is exactly integrable for USF. Finally, these results have been used to give a simple, positive-definite model of the distribution function for USF.

ACKNOWLEDGMENTS

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APPENDIX A: THE ENSKOG COLLISION OPERATOR

Using the shorthand notation $f(1;t)=f(\vec{q}_1,\vec{p}_1;t)$, the collision operator appearing in the Enskog equation can be written as

$$J[f,f]\equiv\chi\int d\vec{p}_2\overline{T}_-(12)f(1;t)f(2;t)$$
$$\equiv-\sigma^2\chi\int d\vec{p}_2\int d\vec{q}\;\delta(q-\sigma)|\vec{g}\cdot\hat{q}|[\Theta(\vec{g}\cdot\hat{q})b_{12}$$
$$-\Theta(-\vec{g}\cdot\hat{q})]f(1;t)f(2;t) \qquad (A1)$$

where the first line introduces the hard-sphere scattering operator and, in the second line, $\vec{q}=\vec{q}_1-\vec{q}_2$, $\vec{g}=\vec{p}_1-\vec{p}_2$ and the operator b_{12} replaces $\vec{g}$ by its postcollisional value $\vec{g}'=\vec{g}-\hat{q}(\vec{g}\cdot\hat{q})$. The hard-sphere diameter has been explicitly written so as to make clear the relation to the Boltzmann collision operator that is obtained by setting $\sigma=0$ and $\chi=1$. Thus the Boltzmann operator is local in the sense that all spatial arguments are evaluated at the same point; the fact that this is not so for the Enskog operator accounts for the additional shear-rate dependence occurring in the moment equations. It is also clear that since the spatial dependence of the collision operator occurs only through $\vec{q}$ it is translationally invariant. Notice also that this can be arranged into the BGK form, (4.1) by defining

$$\nu=-\sigma^2\chi\int d\vec{p}_2\int d\vec{q}\;\delta(q-\sigma)|\vec{g}\cdot\hat{q}|\Theta(-\vec{g}\cdot\hat{q})f(1;t)f(2;t),$$

$$\phi=\frac{-\int d\vec{p}_2\int d\vec{q}\;\delta(q-\sigma)|\vec{g}\cdot\hat{q}|\Theta(\vec{g}\cdot\hat{q})b_{12}f(1;t)f(2;t)}{\int d\vec{p}_2\int d\vec{q}\;\delta(q-\sigma)|\vec{g}\cdot\hat{q}|\Theta(-\vec{g}\cdot\hat{q})f(1;t)f(2;t)}. \tag{A2}$$

To carry out the calculations, one needs to evaluate the coefficients

$$\begin{aligned}B_{[L][M][N]}&\equiv\rho\chi\langle H_{[L]}(1)\overline{T}_-(12)H_{[N]}(1)H_{[M]}(2)\rangle\\&\equiv\rho\chi\langle H_{[N]}(1)H_{[M]}(2)T_+(12)H_{[L]}(1)\rangle,\end{aligned} \tag{A3}$$

where $T_+(12)$ is the conjugate of the scattering operator $\overline{T}_-(12)$ and is given by

$$\begin{aligned}T_+(12)&=-\sigma^2\int d\vec{q}\;\delta(q-\sigma)\Theta(-\vec{g}\cdot\hat{q})\vec{g}\cdot\hat{q}(b_{12}-1)\\&=\sigma^2\int d\hat{q}\;\Theta(-\vec{g}\,'\cdot\hat{q}-aw)(\vec{g}\,'\cdot\hat{q}-aw)(b_{12}-1),\end{aligned} \tag{A4}$$

with $w=\hat{q}_x\hat{q}_y$. The perturbative expansion of the coefficients then follows from an expansion of this operator. First, expand the momentum transfer operator as

$$\begin{aligned}b_{12}H(\vec{p}\,'_1)&=H[\vec{p}\,'_1-\hat{q}(\vec{g}\cdot\hat{q})]\\&=H[\vec{p}\,'_1-\hat{q}(\vec{g}\,'\cdot\hat{q})-aw\hat{q}]=H[\vec{p}\,'_1-\hat{q}(\vec{g}\,'\cdot\hat{q})]\\&\quad-aw\hat{q}\cdot\frac{\partial}{\partial\vec{c}_2}H[\vec{p}\,'_1-\hat{q}(\vec{g}\,'\cdot\hat{q})]\\&\quad+\frac{1}{2}a^2w^2\hat{q}_r\hat{q}_s\frac{\partial^2}{\partial c_{2r}\partial c_{2s}}H[\vec{p}\,'_1-\hat{q}(\vec{g}\,'\cdot\hat{q})]+\cdots\\&\equiv b'_{12}H(\vec{p}\,'_1)-aw\hat{q}\cdot\frac{\partial}{\partial\vec{c}_2}b'_{12}H(\vec{p}\,'_1)\\&\quad+\frac{1}{2}a^2w^2\hat{q}_r\hat{q}_s\frac{\partial^2}{\partial c_{2r}\partial c_{2s}}b'_{12}H(\vec{p}\,'_1)+o(a)^3\end{aligned} \tag{A5}$$

so that one can write

$$T_+(12)=T_+^{(0)}(12)+aT_+^{(1)}(12)+a^2T_+^{(2)}(12)+o(a)^3, \tag{A6}$$

with

$$T_+^{(0)}(12)=-\sigma^2\int d\hat{q}\;\Theta(-\vec{g}\,'\cdot\hat{q})(\vec{g}\,'\cdot\hat{q})(b'-1),$$

$$\begin{aligned}T_+^{(1)}(12)=-\sigma^2\int d\hat{q}\;\Theta(-\vec{g}\,'\cdot\hat{q})\hat{q}_x\hat{q}_y\Bigg(&(b'-1)\\&-(\vec{g}\,'\cdot\hat{q})\hat{q}_r\frac{\partial}{\partial p'_{2r}}b'\frac{\partial}{\partial p'_{1r}}\Bigg),\end{aligned} \tag{A7}$$

$$\begin{aligned}T_+^{(2)}(12)=-\sigma^2\int d\hat{q}\;\Theta(-\vec{g}\,'\cdot\hat{q}-aw)(\hat{q}_x\hat{q}_y)^2\\\times\left(-2\hat{q}_rb'\frac{\partial}{\partial p'_{1r}}+(\vec{g}\,'\cdot\hat{q})\hat{q}_r\hat{q}_s\frac{\partial^2}{\partial p'_{2r}p'_{2s}}b'\right).\end{aligned}$$

Substituting this into Eq. (A3) gives the desired expansion.

APPENDIX B: PERTURBATIVE EXPANSION OF THE EQUATIONS

Recall the fourth-order equations given in the text:

$$\begin{aligned}&2(a\delta_{xr}\delta_{ys}+\gamma\delta_{rs})(\delta_{rx(i}\delta_{j)s}+\delta_{r(i}A_{j)s})\\&\quad=(D_{ij}+C_{[ij][2']}A_{[2']}+C_{[ij][4']}A_{[4']}\\&\qquad+B_{[ij][2'][2'']}A_{[2']}A_{[2'']}),\\&4(a\delta_{xr}\delta_{ys}+\gamma\delta_{rs})(\delta_{r(i}A_{jlm)s}+3\delta_{r(i}A_{jl}\delta_{m)s})\\&\quad=(D_{ijlm}+C_{[ijlm][2']}A_{[2']}+C_{[ijlm][4']}A_{[4']}\\&\qquad+B_{[ijlm][2'][2'']}A_{[2']}A_{[2'']}),\\&B_{[L][M][N]}\equiv\rho\chi\langle H_{[N]}(1)H_{[M]}(2)T_+(12)H_{[L]}(1)\rangle,\end{aligned} \tag{B1}$$

$$C_{[L][M]}\equiv B_{[L][M][0]}+B_{[L][0][M]},$$

$$D_{[L]}=B_{[L][0][0]}.$$

Given the fact that the coefficients are at least of first order in the shear rate, we see that we need $D_{[2]}$ and $D_{[4]}$ to second order in the shear rate, $C_{[L][M]}$ to first order, and $B_{[2][2'][2'']}$ and $B_{[4][2'][2'']}$ to zeroth order. The general couplings are given in Eq. (A3). The required zeroth order couplings are all given in Ref. [17], except for $C^{(0)}_{\mathbf{24}}=C^{(0)}_{\mathbf{42}}$. The complete set is

$$\frac{1}{\alpha}C^{(0)}_{[ij][2]}A_{[2]}=-3A_{(ij)}, \tag{B2}$$

$$\frac{1}{\alpha}C^{(0)}_{[ij][4]}A_{[4]}=-\frac{6}{7}(3A_{(ijrr)}-\delta_{ij}A_{(rrss)}),$$

$$\frac{1}{\alpha}C^{(0)}_{[ijlm][2]}A_{[2]}=-\frac{6}{7}(3A_{(ij}\delta_{lm)}-A_{rr}\delta_{(ij}\delta_{lm)}),$$

$$\begin{aligned}\frac{1}{\alpha}C^{(0)}_{[ijlm][4]}A_{[4]}=-\frac{229}{42}A_{ijlm}+\frac{43}{28}A_{rr(ij}\delta_{lm)}\\+\frac{5}{28}A_{rrss}\delta_{(ij}\delta_{lm)},\end{aligned}$$

$$\frac{1}{\alpha}B^{(0)}_{[ij][2][2']}A_{[2][2']}=-\frac{3}{14}\left(A_{ri}A_{rj}-\frac{1}{3}\delta_{ij}A_{rs}A_{rs}\right),$$

$$\begin{aligned}\frac{1}{\alpha}B^{(0)}_{[ijlm][2][2']}A_{[2][2']}=\frac{23}{14}A_{(ij}A_{lm)}-\frac{41}{14}A_{r(i}\delta_{jl}A_{m)r}\\+\frac{5}{14}A_{rs}A_{rs}\delta_{(ij}\delta_{lm)},\end{aligned}$$

where $\alpha = (16\sqrt{\pi}/15)\,\rho^2\chi$. The first-order coefficients $C^{(1)}_{mn}$ are only needed in the combination $C^{(1)}_{mn}A^{(1)}_n$ and, as noted in the text, the first-order moments have the form $A^{(1)}_n = 2\,\nu_n a\,\delta_{x(i_1}\cdots\delta_{i_n)y}$, where ν_n is a (shear-independent) constant. It turns out to be convenient to calculate the combination $C^{(1)}_{mn}A^{(1)}_n$ directly. Interestingly, these can be worked out for general n,m and are only nonzero if $m=n-2$ or $m=n$. For the cases of interest, I find

$$C^{(1)}_{[ij][2]}A^{(1)}_{[2]} = a^2\rho\chi\nu_2\frac{8\pi}{105}(-6\,\delta_{ij}+2\,\delta_{xi}\delta_{xj}+2\,\delta_{yi}\delta_{yj}),$$

$$\begin{aligned}C^{(1)}_{[ijlm][2]}A^{(1)}_{[2]} = -a^2\rho\chi\nu_2\frac{96\pi}{315}(2\,\delta_{(ij}\delta_{lm)} - \delta_{x(i}\delta_{jl}\delta_{m)x}\\ - \delta_{y(i}\delta_{jl}\delta_{m)y} + 22\delta_{[xxyy][ijlm]}),\end{aligned} \tag{B3}$$

$$\begin{aligned}C^{(1)}_{[ijlm][4]}A^{(1)}_{[4]} = -a^2\rho\chi\nu_4\frac{32\pi}{315}(11\delta_{(ij}\delta_{lm)} + 2\,\delta_{x(i}\delta_{jl}\delta_{m)x}\\ + 2\,\delta_{y(i}\delta_{jl}\delta_{m)y} + 46\delta_{[xxyy][ijlm]}).\end{aligned}$$

Finally, the local-equilibrium terms are

$$\begin{aligned}D_{ij} = -2a\rho\chi\frac{8\pi}{15}\delta_{x(i}\delta_{j)y} + 2a^2\rho\chi\frac{4\sqrt{\pi}}{105}(\delta_{ij}+2\,\delta_{xi}\delta_{xj}\\ + 2\,\delta_{yi}\delta_{yj}) + o(a^3),\end{aligned} \tag{B4}$$

$$\begin{aligned}D_{ijlm} = a^2\rho\chi\frac{88\sqrt{\pi}}{315}(\delta_{(ij}\delta_{lm)} + 4\,\delta_{x(i}\delta_{jl}\delta_{m)x} + 4\,\delta_{y(i}\delta_{jl}\delta_{m)y}\\ + 8\,\delta_{[xxyy][ijlm]}).\end{aligned}$$

Substituting these into the moment equations and rearranging gives the first-order equations as

$$6\nu_2 + 3\nu_4 = \frac{-15}{8\sqrt{\pi}\rho\chi}\left(1+\frac{4\pi}{15}\rho\chi\right),$$

$$18\nu_2 + 615\nu_4 = 0, \tag{B5}$$

while the second order equations are

$$336\varepsilon_2 + 168\sigma_2 + 24\sigma_4 = 8 + 4\sqrt{\pi}\left(1-\frac{105}{4\rho\chi\pi}\right)\nu_2 - 12\nu_2^2,$$

$$336\varepsilon_3 + 168\sigma_3 + 24\sigma_4 = 8 + 4\sqrt{\pi}\nu_2 - 12\nu_2^2,$$

$$\begin{aligned}144(\varepsilon_2+\varepsilon_3) - 8064\sigma_1 + 2232(\sigma_2+\sigma_3) + 240\sigma_4\\ = -4 - 120\nu_2^2 + 48\sqrt{\pi}\nu_2 + 264\sqrt{\pi}a\,\nu_4,\end{aligned}$$

$$\begin{aligned}-432\varepsilon_2 - 14\,760\sigma_2 + 1032\sigma_4 = -16 + 492\nu_2^2 - 24\sqrt{\pi}\nu_2\\ + 48\sqrt{\pi}\left(1+\frac{315}{4\rho\chi\pi}\right)\nu_4,\end{aligned}$$

$$\begin{aligned}-432\varepsilon_3 - 14\,760\sigma_3 + 1032\sigma_4 = -16 + 492\nu_2^2 - 24\sqrt{\pi}\nu_2\\ + 48\sqrt{\pi}\nu_4,\end{aligned}$$

$$\begin{aligned}-21\,984\sigma_4 = -32 + 528\sqrt{\pi}\left(1+\frac{315}{44\rho\chi\pi}\right)\nu_2 - 1104\nu_2^2\\ + 1104\sqrt{\pi}\nu_4.\end{aligned} \tag{B6}$$

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