Divergence of the Chapman-Enskog Expansion

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The Chapman-Enskog expansion for a fluid in uniform shear flow is investigated with use of a Bhatnagar-Gross-Krook model for the nonlinear Boltzmann equation. It is shown that an expansion of the pressure tensor in powers of the uniformity parameter (the shear rate) about the origin does not converge for hard spheres. However, a convergent expansion about the point at infinity can be used to establish that this Chapman-Enskog expansion is asymptotic.

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One of the most successful applications of nonequilibrium statistical mechanics is the calculation of transport coefficients for a simple fluid. These are the coefficients in an expansion of the average fluxes of energy, momentum, etc., in powers of appropriate uniformity parameters (e.g., temperature gradient, velocity gradient). For a low-density gas this expansion is generated from the Chapman-Enskog solution to the Boltzmann equation.[1] To lowest order (Navier-Stokes) the average fluxes have the familiar forms of Newton's viscosity law, Fourier's law of heat conduction, and Fick's diffusion law. The Navier-Stokes coefficients calculated in this way are in excellent agreement with experiment for a wide range of gases and their mixtures. Higher-order terms in the Chapman-Enskog expansion presumably provide successively better approximations for the average fluxes, and characterize the conditions under which the Navier-Stokes forms are a good approximation. However, in spite of its long history and obvious importance, there appear to be few exact results bearing on the convergence of the Chapman-Enskog expansion. The first is due to Ikenberry and Truesdell[2] for a gas of Maxwell molecules (inverse fourth-power potential) in uniform shear flow. They find an explicit expression for the average stress tensor as a function of the shear rate that is analytic about the origin. A second example is due to McLennan[3] for a general class of cutoff potentials. He proves convergence of the Chapman-Enskog expansion for the *linearized* Boltzmann equation. Finally, there is a quite general discussion by Grad[4] that indicates that the expansion is at least asymptotic.

The existing evidence, both experimental and theoretical, therefore suggests that the Chapman-Enskog expansion provides a well-behaved representation of the macroscopic fluxes for a nonequilibrium gas. However, Grad's analysis leaves open the possibility that the expansion actually could be divergent,[5] although sufficiently asymptotic to explain experimental verification of Navier-Stokes–order results. In such a case the relevance of higher-order transport coefficients (e.g., Burnett, super-Burnett, etc.) and the full Chapman-Enskog distribution function itself would be questionable. The purpose of this Letter is to show that the Chapman-Enskog expansion for a very simple physical model is in fact divergent but asymptotic, except in the limits considered by Ikenberry and Truesdell and by McLennan.

The system considered is a simple gas in uniform shear flow.[6] The macroscopic state is characterized by a uniform temperature and density, and a local velocity field given by

$$u_i(r)=a_{ij}r_j, \quad a_{ij}=a\delta_{ix}\delta_{jy}, \tag{1}$$

representing a flow along the x axis with the constant gradient along the y axis. For this simple state the only uniformity parameter is the shear rate, a, and the only nontrivial flux is that for the average momentum. The latter is determined from the pressure tensor, defined by

$$P_{ij}=\int d^3v\, m(v_i-u_i)(v_j-u_j)f(\mathbf{r},\mathbf{v},t), \tag{2}$$

where $f(\mathbf{r},\mathbf{v},t)$ is the one-particle distribution function satisfying the nonlinear Boltzmann equation. The hydrostatic pressure is related to the pressure tensor by $p=P_{ii}/3$, and conservation of energy implies the relationship

$$\partial p/\partial t=-\tfrac{2}{3}a_{ij}P_{ij}. \tag{3}$$

Except for the case of Maxwell molecules, the Boltzmann equation is too difficult to solve, and so we can consider instead a model equation suggested by Bhatnagar, Gross, and Krook[1] (BGK),

$$(\partial/\partial t+\mathbf{v}\cdot\nabla)f=-\zeta(f-f_L). \tag{4}$$

Here, f_L is the local equilibrium distribution function defined in the usual way such that the first five moments of f and f_L are equal. Also, ζ is an average collision frequency independent of velocity but generally a functional of f through its dependence on pressure. The simplest case corresponds to a potential of the form r^{-n}, for which $\zeta \propto p^\alpha$ with $\alpha=(n-4)/2n$. In the following only this case is considered. The BGK model preserves the most important properties of the Boltzmann equation, such as the equilibrium solution and the conservation laws. It is a highly nonlinear equation, through the functional dependence of ζ and the parameters of f_L on f.

The Chapman-Enskog expansion generates a special solution to (4) such that all of the time dependence occurs through $p(t)$. (It is perhaps more usual to use the temperature; however, for the special state considered here the temperature is proportional to the pressure.) The distribution function can be written, therefore, as

$$f(\mathbf{r},\mathbf{v},t)=g(\mathbf{V},p(t);a^*), \tag{5}$$

where $\mathbf{V}=\mathbf{v}-\mathbf{u}$ and $a^*=a/\zeta$. Substitution of (5) into the BGK equation and elimination of the time derivative by use of (3) provides a differential equation for the Chapman-Enskog solution:

$$\left[1+\tfrac{2}{3}a_{ij}^*P_{ij}^*\alpha a^*\frac{\partial}{\partial a^*}-a_{ij}^*V_i\frac{\partial}{\partial V_j}\right]g=g_L. \tag{6}$$

Here, $P_{ij}^*=P_{ij}/p$ is a dimensionless form of the pressure tensor. An equation for P_{ij}^* follows immediately from the definition (2) and Eq. (6):

$$\left[1+\tfrac{2}{3}a_{kl}^*P_{kl}^*\alpha a^*\frac{\partial}{\partial a^*}\right]P_{ij}^*+a_{ik}^*P_{kj}^*+a_{jk}^*P_{ki}^*-\tfrac{2}{3}a_{kl}^*P_{kl}^*P_{ij}^*=\delta_{ij}. \tag{7}$$

Equations (7) are a closed set of equations for the pressure tensor, whose solution specifies all of the parameters of (6) for determination of the Chapman-Enskog distribution function. Finally, expansion of this distribution function in powers of a^* yields the representation obtained from the usual Chapman-Enskog method.

Convergence of the Chapman-Enskog expansion can be determined from the existence of series solutions to Eqs. (6) and (7). Here, attention will be limited to an investigation of the series solution for P_{xy}^*. This component of the pressure tensor is proportional to the nonlinear shear viscosity, $\eta(a)$, and is therefore one of the most important physical properties of uniform shear flow. Furthermore, as a second moment of the distribution function it provides an indirect study of the series solution for (6) as well. Following Zwanzig,[7] a closed nonlinear second-order differential equation for P_{xy}^* is obtained from the set of Eqs. (7),

$$\tfrac{8}{9}\alpha^2z^4\psi(\psi^2)''-\tfrac{4}{3}\alpha z^2[1+2z(\tfrac{1}{2}-\alpha)\psi](\psi^2)'+[1+\tfrac{2}{3}(2-\alpha)z\psi+\tfrac{8}{9}(\tfrac{1}{2}-\alpha)(1-\alpha)z^2\psi^2]\psi=1, \tag{8}$$

where $\psi=-P_{xy}^*(a^*)/a^*\equiv\eta(a)/\eta(0)$, and $z=a^{*2}$. Consider first the case of Maxwell molecules, for which $\alpha=0$. Equation (8) then reduces to an algebraic equation whose real solution is[7]

$$\psi(z)=(2/z)\sinh^2[\tfrac{1}{6}\cosh^{-1}(1+9z)].$$

This result is analytic in the region $|z|<\frac{2}{9}$. The Chapman-Enskog expansion therefore converges for Maxwell molecules.

For potentials with other power laws ($\alpha\neq0$) a closed-form solution is not known and we look for a solution of the form

$$\psi(z)=\sum_{m=0}^{\infty}c_mz^m. \tag{9}$$

By inserting this into Eq. (8) one gets a nonlinear recursive relation for the coefficients c_m, which can be solved numerically. We have considered in detail only hard spheres ($\alpha=\frac{1}{2}$) and all of the following results refer to that case. Table I shows the first ten coefficients. Up to $m=7$ they behave regularly, but from $m=8$ their absolute values increase rapidly. A computer program was used to generate as many coefficients as allowed by the maximum size of a variable in our computer ($\pm10^{\pm4932}$). In Fig. 1 we plot $\mathrm{sgn}(c_m)\ln(|c_m|/m!)$ for $m=5,10,15,\ldots$. (Note that $|c_m|\leq m!$ for all m so that positive values correspond to $c_m<0$ and vice versa.) Two systematic features are

TABLE I. First coefficients in the expansion of the reduced shear viscosity ψ in powers of z (c_m) and in powers of $z^{-1/3}$ ($\bar{c}_m$).

m	c_m	$\bar{c}_m$
0	1	1.13
1	−1	−0.708
2	0.667	0.0871
3	0.778	0.0220
4	−0.815	3.51×10^{-3}
5	−3.83	-3.99×10^{-4}
6	−4.72	-5.95×10^{-4}
7	7.03	-2.63×10^{-4}
8	61.3	-6.06×10^{-5}
9	269.8	5.67×10^{-6}
10	1107.1	1.32×10^{-5}

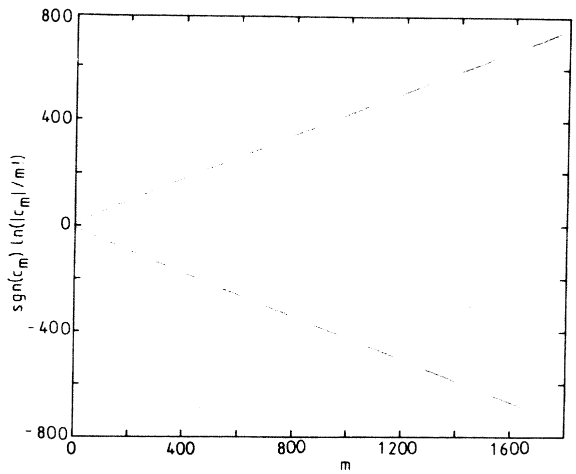

FIG. 1. Behavior of the coefficients c_m in the expansion of the shear viscosity ψ in powers of the square of the shear rate. Only the points corresponding to $m=5$, 10, 15,... are plotted.

observed from these data: (i) The coefficients c_m can be grouped in blocks of increasing size, representing consecutive values with the same sign. Moreover, after $m=24$, the length of a block exceeds that of the preceding block by exactly five. (ii) The points fit very well to two straight lines with the same slope, implying the form

$$|c_m| \cong A\lambda^m m!. \tag{10}$$

We have estimated $\lambda=\frac{2}{3}$ and $A\sim 5\times 10^8$. The behavior given by Eq. (10) implies that the series (9) diverges for all z. Consequently, the Chapman-Enskog expansion of the shear viscosity is divergent in the BGK model for hard spheres.

A divergent series can nevertheless be useful for estimation of the shear viscosity if it is asymptotic. To establish this we have also studied an expansion about the point at infinity given by

$$\psi(z)=z^{-2/3}\sum_{m=0}^{\infty}\bar{c}_m z^{-m/3}. \tag{11}$$

The coefficients for the first few terms in this series are also given in Table I. These coefficients change sign every four or five terms, and the behavior for large m is given approximately by

$$|c_m| \cong \bar{A}\bar{\lambda}^m, \tag{12}$$

with $\bar{\lambda}=3^{-2/3}$ and $\bar{A}\sim 10^{-4}$. In contrast to the expansion (9), the series (11) is convergent[8] for $|z|>\bar{\lambda}^3=\frac{1}{9}$, or $a^*>\frac{1}{3}$. Figure 2 shows $\psi(z)$ as obtained from the series (11) for $\frac{1}{9}<z<1$. Also shown are the partial sums of the Chapman-Enskog expansion (9),

$$\psi^{(N)}(z)\equiv\sum_{m=0}^{N}c_m z^m, \tag{13}$$

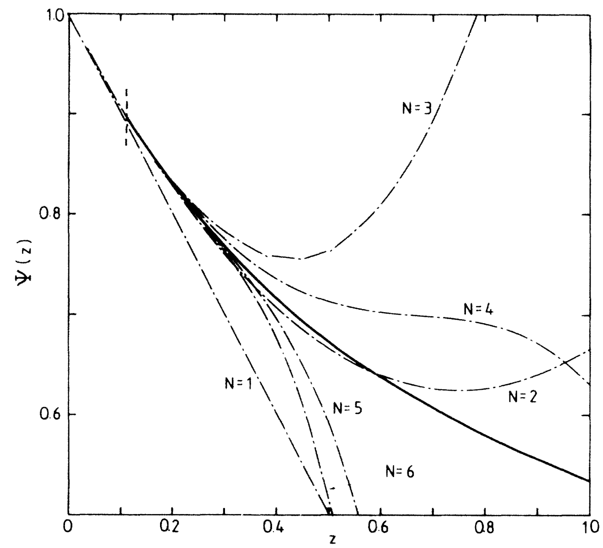

FIG. 2. Reduced shear viscosity $\psi(z)$ as obtained from the expansion in powers of $z^{-1/3}$ (solid line). The broken vertical line indicates the location of the radius of convergence. The truncated series in powers of z, $\psi^{(N)}(z)$, for $N=1,\ldots,6$, are also shown.

for $N=1,\ldots,6$. Except for the super-Burnett order $N=1$, the partial sums match well to $\psi(z)$ at $z=\frac{1}{9}$. This confirms the expectation of Grad that the series is asymptotic. For a given N, the partial sum can be made arbitrarily accurate by decreasing z; however, for fixed z the approximation is not necessarily improved by increasing N.

In summary, the nonlinear BGK equation for hard spheres leads to a divergent but asymptotic Chapman-Enskog expansion for the pressure tensor, when applied to a fluid under uniform shear flow. Although the analysis here was limited to hard spheres, we expect that the same conclusions apply for the class of power-law potentials since the expansion coefficients in (9) should be continuous functions of α, except at the singular value for Maxwell molecules, $\alpha=0$ [the value for which the coefficients of the derivatives in (8) vanish].

It is difficult to determine if this divergence is an artifact of the BGK model or whether it is truly representative of the Boltzmann equation itself. For example, McLennan's proof of convergence for the *linearized* Boltzmann equation does not apply to the linearized BGK model in general.[9] It is possible, then, to have convergence of the linearized Chapman-Enskog solution to the Boltzmann equation while the corresponding solution for the BGK model could diverge. However, the transport properties for the special state of uniform shear flow considered here are intrinsically *nonlinear* beyond Navier-Stokes order (since higher-order derivatives of the velocity field vanish, the linearized Chapman-Enskog expansion is trivially convergent). It is reasonable to conjecture, therefore, that the divergence found here is a property of the nonlinear Boltzmann equation as well.

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[5]It is sometimes argued that the Chapman-Enskog expansion may not exist because of difficulties in matching arbitrary initial and boundary conditions. Such arguments are not compelling, however, since they apply as well to the convergent example of McLennan. See G. Scharf, Helv. Phys. Acta **42**, 5 (1969).

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[8]The finite radius of convergence indicates a singularity in the complex plane on the circle $|z|=\frac{1}{9}$. We have used the coefficients $\bar{c}_m$ (up to $m=14\,637$) to estimate the expansion in powers of $z^{-1/3}-z_0^{-1/3}$ for $z_0=0.5, 1.0$, and 1.5. The results indicate that the singularity lies on the real axis.

[9]The key inequality (22) of Ref. 3 does not apply when the *unbounded* linearized Boltzmann operator is replaced by the *bounded* linearized BGK operator.