Nonequilibrium entropy of a sheared gas

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Abstract

The nonequilibrium entropy of a dilute gas under uniform shear flow is analyzed in terms of an expansion in powers of the shear rate. To this end, the Boltzmann equation for Maxwell molecules is exactly solved to super-Burnett order, the next two orders being also partially obtained. This allows us to get the entropy through sixth order in the shear rate. Comparison with results obtained from the Bhatnagar-Gross-Krook kinetic model indicates that the latter gives a smaller entropy than the Boltzmann equation.

1. Introduction

Needless to say, the entropy is a fundamental concept in equilibrium thermodynamics. Near equilibrium, Prigogine's principle of minimum entropy production [1] shows that the linear constitutive equations in steady states can be obtained from a local equilibrium entropy function. In extended irreversible thermodynamics [2], the entropy is further extended to allow for a functional dependence on the fluxes. Nevertheless, no general consensus about how to define nonequilibrium entropy exists. This is a crucial point in the distinction between a thermodynamic and a kinetic temperature far from equilibrium [3-5].

In the case of a low-density gas, there is no question as to what the proper definition of nonequilibrium entropy is. It is given by [6]:

$$S = -k_B \int d\mathbf{r} \int d\mathbf{v} \, f \log f + \text{const.}, \tag{1.1}$$

where k_B is the Boltzmann constant and $f(\mathbf{r}, \mathbf{v}; t)$ is the one-particle velocity distribution function. The latter is the solution to the Boltzmann equation:

$$\frac{\partial}{\partial t} f + \mathbf{v} \cdot \nabla f = \int d\mathbf{v}_1 \int d\Omega \, g\sigma(g, \cos\theta) [f_1' f' - f_1 f] \equiv J[f, f]. \tag{1.2}$$

We note that, even for a low-density gas, the evaluation of the entropy is quite a difficult task. First, one has to solve Eq. (1.2) with the appropriate initial and boundary conditions; next, one must perform the space and velocity integrations in Eq. (1.1). In order to get explicit results, we focus in this paper on a given state and a given interaction and follow a perturbation approach. Among all possible nonequilibrium states, we select here the so-called uniform shear flow, which is perhaps one of the most extensively studied from a theoretical point of view as well as in simulations [7]. For this state, Eq. (1.2) lends itself to an exact analysis by the moment method if one specializes to Maxwell molecules, i.e., particles interacting via a repulsive r^{-4} potential. Equivalently, the velocity-dependent coefficients of the expansion of the distribution function in powers of the shear rate can be exactly obtained. In this paper, we follow that method to get the entropy through sixth order in the shear rate.

The uniform shear flow state is described in Section 2. By expanding in powers of the shear rate, the Boltzmann equation decouples into a hierarchy of equations, one for each order, that can be solved in a recursive way. Such a hierarchy is explicitly solved in Section 3 to get the velocity distribution function through super-Burnett order, the projection of the fourth-order term onto the subspace spanned by polynomials of degree 2 and 4, and the projection of the fifth-order term onto the subspace spanned by polynomials of degree 2. All these terms are needed in the evaluation of the entropy through sixth order in the shear rate, the results being discussed in Section 4. It is shown there that, at least for small shear rates, the solution of the Boltzmann equation has a smaller entropy than that of the Bhatnagar-Gross-Krook (BGK) equation. Padé approximants suggest that this trend could also extend to large shear rates.

2. Entropy of the uniform shear flow

The uniform shear flow state is characterized by a constant density n, a spatially uniform temperature T and a linear flow velocity field $\mathbf{u}(\mathbf{r}) = ay\hat{\mathbf{x}}$, a being the constant shear rate. At a kinetic level, the uniform shear flow is described by a solution to Eq. (1.2) of the form $f(\mathbf{r}, \mathbf{v}; t) = f(\mathbf{V}; t)$, $\mathbf{V} \equiv \mathbf{v} - \mathbf{u}(\mathbf{r})$. In that case, Eq. (1.2) becomes [8,9]

$$\frac{\partial}{\partial t} f - aV_y \frac{\partial}{\partial V_x} f = J[f, f]. \tag{2.1}$$

The temperature $T(t)$ increases in time due to viscous heating effects. This can be accounted for by the introduction of a (Gaussian) thermostat force $\mathbf{F} = -ma\mathbf{V}$ [7]. In the special case of Maxwell molecules, the collision rate $g\sigma(g, \cos\theta) = \sigma_0(\cos\theta)$ is independent of the relative velocity g and an exact relationship holds between the solution to Eq. (2.1) with and without a thermostat [8,9]. More specifically, if we define

$$\xi = (m/2k_BT)^{1/2} \mathbf{V}, \tag{2.2}$$

$$\phi(\xi) = (1/n) \left(m/2k_B T\right)^{-3/2} f(\mathbf{V}),$$ (2.3)

Eq. (2.1) reduces to

$$\frac{\partial}{\partial t}\phi - a\xi_y \frac{\partial}{\partial \xi_x}\phi - \alpha(a)\frac{\partial}{\partial \xi} \cdot \xi\phi = nJ[\phi,\phi],$$ (2.4)

where the thermostat parameter α for long times is

$$\alpha(a) = \frac{2}{3}\, \nu\, \sinh^2\left\{\frac{1}{6}\cosh^{-1}\left[1 + 9\left(\frac{a}{\nu}\right)^2\right]\right\}.$$ (2.5)

In Eq. (2.5), $\nu \equiv \lambda_{02}n$ is an effective collision frequency, λ_{02} being an eigenvalue of the linearized collision operator (see below). Henceforth, we will take $\nu^{-1} = 1$ as the unit of time. The exact equivalence between Eqs. (2.1) and (2.4) for Maxwell molecules allows us to map the long-time solution of Eq. (2.1) into the stationary solution of Eq. (2.4). We focus now on such a solution and discard the term $\partial\phi/\partial t$ in Eq. (2.4). In addition, Eq. (2.4) is invariant under the following transformations:

$$\phi(\xi_x,\xi_y,\xi_z;a) = \phi(-\xi_x,-\xi_y,\xi_z;a)$$ (2.6a)

$$= \phi(\xi_x,\xi_y,-\xi_z;a)$$ (2.6b)

$$= \phi(-\xi_x,\xi_y,\xi_z;-a).$$ (2.6c)

Despite the specialization to Maxwell molecules, the explicit solution of Eq. (2.4) for arbitrary shear rate a is not known. On the other hand, the second degree [10] and fourth degree [9] moments of ϕ are exactly known. It must be noticed that, even if $\phi(\xi;a)$ were known, an explicit expression of the nonequilibrium entropy, Eq. (1.1), as a function of the shear rate would not possibly be feasible. For instance, the solution of Eq. (2.4) in the BGK approximation, i.e.,

$$J[\phi,\phi] \rightarrow -\lambda_{02}[\phi - \pi^{-3/2}\exp(-\xi^2)],$$ (2.7)

is known [11] but still the entropy has to be obtained by expanding in powers of the shear rate [3].

As said in Section 1, the aim of this paper is to evaluate the entropy through sixth order in the shear rate. Let us define the reduced excess entropy per particle

$$S(a) \equiv (S - S_{\mathrm{eq}})/Nk_B = -\int d\xi\; \phi(\xi;a)\; \log\frac{\phi(\xi;a)}{\phi_0(\xi)},$$ (2.8)

where $\phi_0(\xi) = \phi(\xi;0) = \pi^{-3/2}\exp(-\xi^2)$ is the local equilibrium distribution function. A useful representation of ϕ is obtained by considering the following set of basis functions:

$$\Psi_{\mathbf{k}}(\xi) \equiv \Psi_{r\ell m}(\xi) = \left(2\pi^{3/2}\frac{r!}{\Gamma(r+\ell+3/2)}\right)^{1/2} \xi^\ell\, L_r^{\ell+1/2}(\xi^2)\, Y_\ell^m(\widehat{\xi}),$$ (2.9)

where in the spherical harmonics the polar angle is taken with respect to the z direction and the azimuthal angle with respect to the x direction. The functions $\{\Psi_k(\xi)\}$ constitute an orthonormal set with the inner product

$$\langle \chi_1 | \chi_2 \rangle = \int d\xi \, \phi_0(\xi) \, \chi_1^*(\xi) \, \chi_2(\xi). \tag{2.10}$$

Now we represent the velocity distribution function $\phi(\xi; a)$ in terms of the set $\{\Psi_k(\xi)\}$:

$$\phi(\xi; a) = \phi_0(\xi) \sum_k M_k(a) \Psi_k(\xi), \tag{2.11}$$

$$M_k(a) = \langle \Psi_k | \phi / \phi_0 \rangle. \tag{2.12}$$

According to the invariance properties (2.6a) and (2.6b), $M_k(a) = 0$ if ℓ and/or m are odd. Insertion of Eq. (2.11) into Eq. (2.4) yields a hierarchy of algebraic moment equations that, in principle, can be recursively solved to get the moments $M_k(a)$. Very recently, it has been shown [9,12,13] that the moments of degree $k \equiv 2r + \ell \geq 4$ diverge for shear rates larger than a critical value $a_c^{(k)}$ that decreases as k increases. For instance, $a_c^{(4)} = 6.846$, $a_c^{(6)} = 2.346$.

Since an explicit closed expression for ϕ does not seem feasible, we look for a perturbation solution. By expanding the moments in powers of a, Eq. (2.11) can be recast into the form

$$\phi(\xi; a) = \phi_0(\xi) \left(1 + \sum_{n=1}^{\infty} \Phi^{(n)}(\xi) \, a^n \right). \tag{2.13}$$

This is nothing else but the Chapman-Enskog expansion [6] particularized to the uniform shear flow. Since the expansion of M_k cannot converge for $a > a_c^{(k)}$ and $a_c^{(k)} \overset{k \to \infty}{\longrightarrow} 0$ [13], the expansion (2.13) is expected to be only asymptotic. Substitution of Eq. (2.13) into Eq. (2.4) gives

$$\Phi^{(n-1)} \xi_y \frac{\partial}{\partial \xi_x} \log \phi_0 + \xi_y \frac{\partial}{\partial \xi_x} \Phi^{(n-1)}$$

$$+ \sum_{n'=2}^{n} \alpha^{(n')} \left(\Phi^{(n-n')} \xi \cdot \frac{\partial}{\partial \xi} \log \phi_0 + \frac{\partial}{\partial \xi} \cdot \xi \Phi^{(n-n')} \right)$$

$$= \lambda_{02}^{-1} I \Phi^{(n)} + \lambda_{02}^{-1} \sum_{n'=1}^{n-1} K[\Phi^{(n')}, \Phi^{(n-n')}], \tag{2.14}$$

where K is the bilinear operator

$$K[\chi_1, \chi_2] \equiv -(1/\phi_0) J[\phi_0 \chi_1, \phi_0 \chi_2]$$

$$= \int d\xi_1 \int d\Omega \, \sigma_0(\cos\theta) \phi_0(\xi_1) [\chi_1(\xi) \chi_2(\xi_1) - \chi_1(\xi') \chi_2(\xi_1')], \tag{2.15}$$

I is the linear operator

$$I\chi = K[\chi, 1] + K[1, \chi],\tag{2.16}$$

and $\alpha^{(n)}$ are the coefficients of the expansion of α, Eq. (2.5) in powers of a: $\alpha^{(0)} = \alpha^{(1)} = \alpha^{(3)} = \alpha^{(5)} = \cdots = 0$, $\alpha^{(2)} = \frac{1}{3}$, $\alpha^{(4)} = -\frac{4}{9}, \cdots$. It must be noticed that the basis functions $\{\Psi_{\mathbf{k}}(\boldsymbol{\xi})\}$ are eigenfunctions of the operator I [14,15]:

$$I\Psi_{r\ell m}(\boldsymbol{\xi}) = \lambda_{r\ell}\Psi_{r\ell m}(\boldsymbol{\xi}),\tag{2.17}$$

$$\lambda_{r\ell} = \int d\Omega\, \sigma_0(\cos\theta)$$

$$\times [\, 1 + \delta_{r0}\delta_{\ell0} - \cos^{2r+\ell}(\tfrac{1}{2}\theta)\, P_\ell(\cos(\tfrac{1}{2}\theta)) - \sin^{2r+\ell}(\tfrac{1}{2}\theta)\, P_\ell(\sin(\tfrac{1}{2}\theta))\,].$$
$$\tag{2.18}$$

It is easy to check by induction that $\Phi^{(n)}(\boldsymbol{\xi})$ is a polynomial in $\boldsymbol{\xi}$ of degree $2n$. Consequently, $\Phi^{(n)}(\boldsymbol{\xi})$ can be expressed as a linear combination of a *finite* number of eigenfunctions:

$$\Phi^{(n)}(\boldsymbol{\xi}) = \sum_{\substack{\mathbf{k} \\ 2\le k\le 2n}} M_{\mathbf{k}}^{(n)}\Psi_{\mathbf{k}}(\boldsymbol{\xi}).\tag{2.19}$$

This exact property is peculiar of the Maxwell interaction. From Eqs. (2.12), (2.13), and (2.19) one gets

$$M_{\mathbf{k}}(a) = \sum_{n=k/2}^{\infty} M_{\mathbf{k}}^{(n)}a^n.\tag{2.20}$$

On account of the invariance property (2.6c), $M_{r\ell m}^{(n)} = (-1)^n M_{r\ell\,-m}^{(n)}$. As a consequence,

$$\langle \Phi^{(n)}|\Phi^{(n')}\rangle = \sum_{\substack{\mathbf{k} \\ 2\le k\le \min(2n,2n')}} M_{\mathbf{k}}^{(n)*}M_{\mathbf{k}}^{(n')},\tag{2.21}$$

which vanishes if $n + n' = \text{odd}$.

Thus, in order to know $\phi(\boldsymbol{\xi}; a)$ through order n in a we need to determine the coefficients $\{M_{\mathbf{k}}^{(n')}, k \le 2n', n' \le n\}$. However, the knowledge of a much smaller number of coefficients suffices to know $\mathcal{S}(a)$ through order n:

$$\mathcal{S}(a) = -\langle \phi/\phi_0 | \log(\phi/\phi_0)\rangle = \sum_{n=2,4,6,\ldots} \mathcal{S}^{(n)}a^n.\tag{2.22}$$

The expressions for $\mathcal{S}^{(2)}$, $\mathcal{S}^{(4)}$, and $\mathcal{S}^{(6)}$ are

$$\mathcal{S}^{(2)} = -\tfrac{1}{2}\langle \Phi^{(1)}|\Phi^{(1)}\rangle,\tag{2.23}$$

$$\mathcal{S}^{(4)} = -\tfrac{1}{12}\langle \Phi^{(1)}|\Phi^{(1)^3}\rangle + \tfrac{1}{2}\langle \Phi^{(2)}|\Phi^{(1)^2} - \Phi^{(2)}\rangle - \langle \Phi^{(3)}|\Phi^{(1)}\rangle,\tag{2.24}$$

$$\mathcal{S}^{(6)} = -\tfrac{1}{30}\langle \Phi^{(1)}|\Phi^{(1)^5}\rangle + \tfrac{1}{12}\langle \Phi^{(2)}|3\Phi^{(1)^4} - 6\Phi^{(1)^2}\Phi^{(2)} + 2\Phi^{(2)^2}\rangle$$

$$-\tfrac{1}{6}\langle \Phi^{(3)} | 2\Phi^{(1)^3} - 6\Phi^{(1)}\Phi^{(2)} + 3\Phi^{(3)}\rangle$$

$$+\tfrac{1}{2}\langle \Phi^{(4)} | \Phi^{(1)^2} - 2\Phi^{(2)}\rangle - \langle \Phi^{(5)} | \Phi^{(1)}\rangle. \tag{2.25}$$

In general, $S^{(n)}$ is a linear combination of terms of the form $\langle \Phi^{(n')} | P_{2(n-n')}\rangle$, where $P_{2(n-n')}(\xi)$ is a polynomial in ξ of degree $2(n-n')$ and $1 \le n' \le n-1$. From Eq. (2.20) then follows that only the coefficients $M_k^{(n')}$ with $2 \le k \le \min(2n', 2n - 2n')$ contribute to $S^{(n)}$. This is illustrated in Fig. 1. In particular, to calculate $S^{(2)}$, $S^{(4)}$, and $S^{(6)}$, we need $\Phi^{(1)}$, $\Phi^{(2)}$, $\Phi^{(3)}$, the projection of $\Phi^{(4)}$ onto the subspace spanned by $\{\Psi_k(\xi), k = 2, 4\}$ and the projection of $\Phi^{(5)}$ onto the subspace spanned by $\{\Psi_k(\xi), k = 2\}$. These functions are derived in the next section.

3. Perturbation expansion of the distribution function

The solution of Eq. (2.14) is

$$\Phi^{(n)} = \lambda_{02} l^{-1} \left[-2\xi_x\xi_y \Phi^{(n-1)} + \xi_y \frac{\partial}{\partial \xi_x} \Phi^{(n-1)} \right.$$

$$\left. + \sum_{n'=2}^{n} \alpha^{(n')} \left(-2\xi^2 \Phi^{(n-n')} + \frac{\partial}{\partial \xi} \cdot \xi \Phi^{(n-n')} \right) - \lambda_{02}^{-1} \sum_{n'=1}^{n-1} K[\Phi^{(n')}, \Phi^{(n-n')}] \right].$$
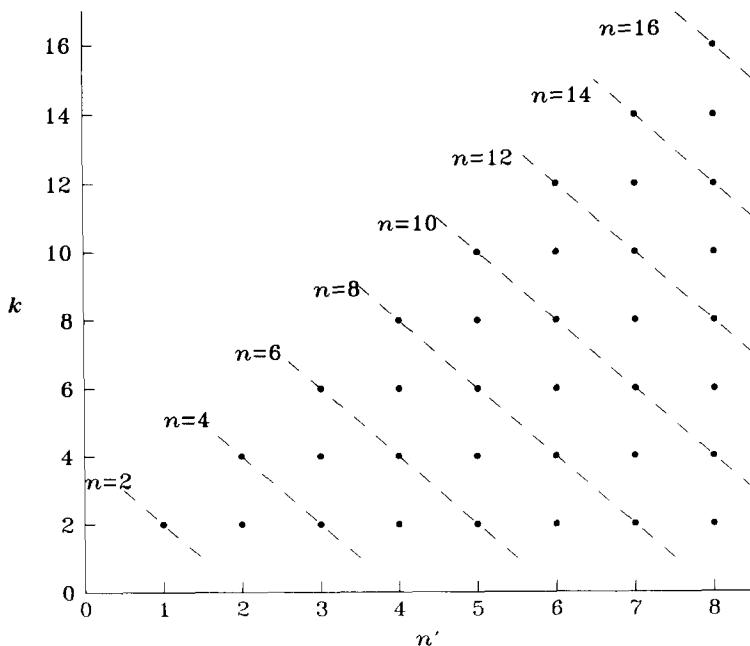
$$\tag{3.1}$$

Fig. 1. Each dot in this diagram represents all the coefficients $M_{r\ell m}^{(n')}$ of the same degree $k \equiv 2r + \ell$ and order n'. Only the coefficients lying below the line $n = $ const. are required to evaluate the entropy through order n.

The expression enclosed between braces is a polynomial of degree $2n$. Once it is expressed as a linear combination of $\{\Psi_k, k \leq 2n\}$, the action of the operator I^{-1}, on account of Eq. (2.17), is straightforward and one gets $\Phi^{(n)}$. The process can be continued recursively. The first step is obtained by making $n = 1$ in Eq. (3.1):

$$\Phi^{(1)}(\xi) = -2\xi_x\xi_y = -\Psi_{022}^{(-)}(\xi), \tag{3.2}$$

where we have called

$$\Psi_{r\ell m}^{(\pm)}(\xi) = \frac{\exp[(i\pi/4)(-1 \pm 1)]}{\sqrt{2}}[\Psi_{r\ell m}(\xi) \pm \Psi_{r\ell -m}(\xi)]. \tag{3.3}$$

Substitution of Eq. (3.2) into Eq. (3.1) with $n = 2$ yields

$$\Phi^{(2)} = \lambda_{02}I^{-1}\{4\xi_x^2\xi_y^2 - 2\xi_y^2 + 1 - \tfrac{2}{3}\xi^2 - \lambda_{02}^{-1}K[\Phi^{(1)}, \Phi^{(1)}]\}. \tag{3.4}$$

A tedious but straightforward calculation gives

$$
\begin{aligned}
K[\Phi^{(1)}, \Phi^{(1)}] ={}& -\tfrac{2}{15}\lambda_{02}[\xi^4 - 5\xi^2(\xi_x^2 + \xi_y^2) + 30\xi_x^2\xi_y^2 + \tfrac{5}{2}(\xi_x^2 + \xi_y^2) - \tfrac{5}{4}] \\
&+ \tfrac{2}{35}\lambda_{04}[\xi^4 - 5\xi^2(\xi_x^2 + \xi_y^2) + 35\xi_x^2\xi_y^2] \\
={}& -\tfrac{2}{15}\lambda_{02}[\tfrac{3\sqrt{105}}{14}\Psi_{040}(\xi) - \tfrac{15\sqrt{3}}{2}\Psi_{044}^{(+)}(\xi) \\
&+ \tfrac{5\sqrt{42}}{42}\Psi_{120}(\xi) - \tfrac{\sqrt{30}}{6}\Psi_{200}(\xi)] \\
&+ \tfrac{2}{35}\lambda_{04}[\tfrac{\sqrt{105}}{4}\Psi_{040}(\xi) - \tfrac{35\sqrt{3}}{4}\Psi_{044}^{(+)}(\xi)].
\end{aligned}\tag{3.5}
$$

After insertion of Eq. (3.5) into Eq. (3.4) one gets

$$
\begin{aligned}
\Phi^{(2)}(\xi) ={}& \Psi_{022}^{(+)}(\xi) - \tfrac{\sqrt{3}}{3}\Psi_{020}(\xi) + \tfrac{\sqrt{105}}{70}(4/\lambda_{04} - 1)\Psi_{040}(\xi) \\
&- \tfrac{\sqrt{3}}{2}(4/\lambda_{04} - 1)\Psi_{044}^{(+)}(\xi) - \tfrac{10\sqrt{42}}{147}\Psi_{120}(\xi) + \tfrac{\sqrt{30}}{6}\Psi_{200}(\xi) \\
={}& (8/35\lambda_{04} + \tfrac{1}{245})\xi^4 - (8/7\lambda_{04} - \tfrac{34}{49})\xi^2(\xi_x^2 + \xi_y^2) \\
&+ \left(8/\lambda_{04} - 2\right)\xi_x^2\xi_y^2 - \tfrac{29}{21}\xi^2 + \tfrac{4}{7}\xi_x^2 - \tfrac{10}{7}\xi_y^2 + \tfrac{5}{4},
\end{aligned}\tag{3.6}
$$

where in the first step we have called $\lambda_{r\ell} \equiv \lambda_{r\ell}/\lambda_{02}$ and have taken into account that $\lambda_{12} = \tfrac{7}{6}$, $\lambda_{20} = \tfrac{2}{3}$. The numerical values of $\lambda_{r\ell}$ can be obtained from Table 1 of Ref. [15]. In particular, $\lambda_{04} \simeq 1.87313$.

Eqs. (3.2) and (3.6) give the velocity distribution function through Burnett order for Maxwell molecules under uniform shear flow. The process can be continued to get higher order contributions. The term $\Phi^{(3)}$ is obtained by inserting Eqs. (3.2) and (3.6) into Eq. (3.1) and performing lengthy calculations. The final result is

$$
\begin{aligned}
\Phi^{(3)} ={}& \tfrac{4}{3}\Psi_{022}^{(-)}(\xi) + \tfrac{\sqrt{21}}{7}(20/7\lambda_{04}^2 + 132/49\lambda_{04} - 1)\Psi_{042}^{(-)}(\xi) \\
&- \sqrt{3}(4/\lambda_{04}^2 + 2/\lambda_{04} - 1)\Psi_{044}^{(-)}(\xi) \\
&+ \tfrac{8\sqrt{14}}{36015}(3402/\lambda_{04} - 193)\Psi_{122}^{(-)}(\xi)
\end{aligned}
$$

$$+ \frac{3}{4} \frac{(4 - \lambda_{04})(4 - 4\lambda_{04} + \lambda_{06})}{\lambda_{04}\lambda_{06}} \left(\frac{\sqrt{22}}{11} \Psi_{062}^{(-)}(\xi) - \sqrt{10}\Psi_{066}^{(-)}(\xi) \right)$$

$$+ \frac{10\sqrt{462}}{539} \frac{33\lambda_{04}^2 - 97\lambda_{04} - 140}{\lambda_{04}(69\lambda_{04} - 49)} \Psi_{142}^{(-)}(\xi)$$

$$+ \frac{\sqrt{14}}{490} \frac{4872\lambda_{04}^2 - 20761\lambda_{04} - 26208}{\lambda_{04}(24\lambda_{04} + 49)} \Psi_{222}^{(-)}(\xi), \tag{3.7}$$

where $\lambda_{06} \simeq 2.45323$. Eqs. (3.2), (3.6), and (3.7) give the velocity distribution function for Maxwell molecules under uniform shear flow through super-Burnett order. They have been used in Ref. [16] to refute an extremum property of the Gaussian thermostat.

The term $\Phi^{(4)}$ is a polynomial of degree 8. Nevertheless, as discussed in Section 2, we only need $\mathcal{P}_4\Phi^{(4)}$ to get $\mathcal{S}^{(6)}$, where we have called

$$\mathcal{P}_k = \sum_{\substack{\mathbf{k}' \\ k' \leq k}} |\Psi_{\mathbf{k}'}\rangle\langle\Psi_{\mathbf{k}'}| \tag{3.8}$$

to be the projection operator onto the subspace spanned by the eigenfunctions of degree equal to or less than k. Thus, when computing $\mathcal{P}_4\Phi^{(4)}$ from Eq. (3.1) we just discard the terms of degrees 6 and 8. The result is

$$\mathcal{P}_4\Phi^{(4)}(\xi) = \frac{2\sqrt{3}}{3}\Psi_{020}(\xi) - 2\Psi_{022}^{(+)}(\xi) + \frac{\sqrt{30}}{77175}(81648/\lambda_{04} - 47507)\Psi_{200}(\xi)$$

$$+ \sqrt{105}\left(\frac{60}{343\lambda_{04}^3} + \frac{23756}{180075\lambda_{04}^2} - \frac{30756}{420175\lambda_{04}} - \frac{1}{210} \right)\Psi_{040}(\xi)$$

$$- \frac{\sqrt{21}}{7}\left(\frac{48}{7\lambda_{04}^3} + \frac{230}{49\lambda_{04}^2} - 1 \right)\Psi_{042}^{(+)}(\xi)$$

$$+ \sqrt{3}\left(\frac{372}{49\lambda_{04}^3} + \frac{24544}{5145\lambda_{04}^2} + \frac{30756}{12005\lambda_{04}} - \frac{11}{6} \right)\Psi_{044}^{(+)}(\xi)$$

$$+ \frac{4\sqrt{42}}{1764735}\left(\frac{66150}{\lambda_{04}^2} + \frac{212058}{\lambda_{04}} - 143977 \right)\Psi_{120}(\xi)$$

$$- \frac{4\sqrt{14}}{49}\left(\frac{18}{\lambda_{04}^2} + \frac{4149}{245\lambda_{04}} - \frac{45191}{5145} \right)\Psi_{122}^{(+)}(\xi). \tag{3.9}$$

Finally, although $\Phi^{(5)}$ is a polynomial of degree 10, only $\mathcal{P}_2\Phi^{(5)}$ is needed. The result is

$$\mathcal{P}_2\Phi^{(5)}(\xi) = -\tfrac{28}{9}\Psi_{022}^{(-)}(\xi). \tag{3.10}$$

4. Discussion

Once the explicit expressions of $\Phi^{(1)}, \Phi^{(2)}, \Phi^{(3)}, \mathcal{P}_4\Phi^{(4)}$, and $\mathcal{P}_2\Phi^{(5)}$ are known, Eqs. (2.23)–(2.25) provide $\mathcal{S}^{(2)}$, $\mathcal{S}^{(4)}$, and $\mathcal{S}^{(6)}$ by just performing Gaussian integrals. The result is

$$\mathcal{S}^{(2)} = -1/2, \tag{4.1}$$

$$\mathcal{S}^{(4)} = -\frac{216}{35\,\lambda_{04}^2} + \frac{216}{35\,\lambda_{04}} - \frac{1632}{1715} \simeq 0.58417, \tag{4.2}$$

$$\mathcal{S}^{(6)} \simeq -1.36502. \tag{4.3}$$

Since the expression of $\mathcal{S}^{(6)}$ in terms of λ_{04} and λ_{06} is rather involved, we have given above only its numerical value for $\lambda_{04} \simeq 1.87313$ and $\lambda_{06} \simeq 2.45323$. It is striking that $\mathcal{S}^{(6)}$ differs from $-4\mathcal{S}^{(4)2}$ in less than 2×10^{-6}, (a value that, however, cannot be accounted for by the error bars of the eigenvalues tabulated in Ref. [15]). While this could be just a coincidence [17], it would be interesting to analyze this point in the future in more detail.

In order to put the results (4.1)–(4.3) in a proper context, let us consider two different approximations. First, in the BGK approximation, cf. Eq. (2.7), the computation of the coefficients of $\mathcal{S}(a)$ is much easier than in the Boltzmann equation. In the former case, Eq. (3.1) still applies, except that the operators become $I \to \lambda_{02}$, $K \to 0$. After performing the corresponding calculations, one gets

$$\begin{aligned}
\mathcal{S}_{\text{BGK}} = &-\frac{1}{2}a^2 + \frac{1}{4}a^4 - \frac{5}{54}a^6 + \frac{153}{8}a^8 + \frac{192\,101}{270}a^{10} + \frac{78\,664\,283}{2916}a^{12} \\
&+ \frac{2\,336\,070\,287}{10\,206}a^{14} - \frac{7\,627\,231\,329\,077}{34\,992}a^{16} - \frac{2\,347\,536\,574\,990\,979}{39\,366}a^{18} \\
&+ O(a^{20}).
\end{aligned} \tag{4.4}$$

The coefficients $\mathcal{S}_{\text{BGK}}^{(2)} = -\frac{1}{2}$ and $\mathcal{S}_{\text{BGK}}^{(4)} = \frac{1}{4}$ were already obtained in Ref. [3], while the remaining coefficients appearing in Eq. (4.4) had not been evaluated before. The equality $\mathcal{S}_{\text{BGK}}^{(2)} = \mathcal{S}^{(2)}$ is a consequence of the fact that the BGK equation coincides with the Boltzmann equation to Navier-Stokes order, Eq. (3.2), for uniform shear flow. The surprising result is that $\mathcal{S}^{(4)} > \mathcal{S}_{\text{BGK}}^{(4)}$. This means that, at least for small shear rates, the nonequilibrium entropy obtained from the Boltzmann equation is *larger* than the one obtained from the BGK model. In other words, the velocity distribution function given by the Boltzmann equation exhibits a less "ordered" structure (in the entropy sense) than the one given by the BGK equation, at least for states not very far from equilibrium. This seems to be rather counter-intuitive if one considers that the BGK model can be viewed as a coarse-grained version of the Boltzmann equation and contains much less information than the latter. We will come back to this point later on.

As a second approach, we now use information theory (IT). According to this method [18], if one only knows a finite number of velocity moments, the distribution function can be approximated by the one that maximizes the entropy, Eq. (2.8), subject to the

constraints imposed by those moments. The corresponding entropy function $S_{IT}(a)$ is then an upper bound of the actual function $S(a)$. If the explicit knowledge of the second degree moments is taken into account, $S_{IT}(a)$ is easily obtained as [3]

$$S_{IT}(a) = \frac{1}{2}\log\frac{1 + 3\alpha(a)}{[1 + 2\alpha(a)]^3}, \tag{4.5}$$

where $\alpha(a)$ is given by Eq. (2.5). The behavior for small shear rates is $S_{IT}(a) = -\frac{1}{2}a^2 + \frac{3}{4}a^4 - \frac{95}{54}a^6 + O(a^8)$. Since the second degree moments obtained from the BGK and Boltzmann equations coincide for any shear rate, it follows that $S_{IT}(a)$ is an upper estimate of both $S(a)$ and $S_{BGK}(a)$. Note that $S_{IT}^{(4)} > S^{(4)} > S_{BGK}^{(4)}$ but $S_{IT}^{(6)} < S^{(6)} < S_{BGK}^{(6)}$.

It is interesting to carry out a broader comparison between the Boltzmann and the BGK entropies by considering Padé approximants of the corresponding power series [19]. Since several approximants are possible, a criterion based on the behavior for large shear rates seems to be adequate for choosing the most reasonable one. The information-theory entropy behaves for large shear rates as $S_{IT} \approx -\frac{2}{3}\log a$. Since $S_{IT}(a)$ is an upper bound of $S(a)$, the simplest behavior compatible with a Padé approximant is $S(a) \sim -a^2$. We will call the function $\overline{S}(a) = -\frac{1}{2}a^2 P_n(a^2)/Q_n(a^2)$, where P_n and Q_n are polynomials of degree n, a Padé approximant (n, n) of the actual function $S(a)$. In the case of the entropy derived from the Boltzmann equation, the results of this paper allow us to construct the Padé (1,1):

$$\overline{S}(a) = -\frac{1}{2}a^2\frac{1 + 2S^{(4)}a^2}{1 + 4S^{(4)}a^4}, \tag{4.6}$$

where we have already taken into account that $S^{(6)} \simeq -4S^{(4)2}$. In the case of the entropy obtained from the BGK model, Eq. (4.4), one can get the Padés (1,1), (2,2), (3,3), and (4,4). Fig. 2 shows the function $-2S(a)/a^2$ in the range $0 < a^2 < 1$ as given by (a) information-theory [Eq. (4.5)], (b) the Padé (1,1) obtained from the Boltzmann equation [Eq. (4.6)], and (c) the Padés (2,2), (3,3), and (4,4) obtained from the BGK equation. The results clearly suggest that $S(a)$ is larger than $S_{BGK}(a)$, not only for small shear rates, but also for quite large values. As commented above, this effect seems to be paradoxical. A possible explanation for it lies in the fact that the entropy function (2.8) is especially sensitive to the details of the distribution function for *thermal* velocities, i.e. $|\xi| \sim 1$. As we have recently observed from a numerical solution of the Boltzmann equation [20], the latter exhibits a smaller distortion for thermal velocities than the analytical solution of the BGK model [11]. On the other hand, the Boltzmann distribution function for large velocities is much more distorted from local equilibrium than the BGK distribution function. In fact, the former seems to develop a high-velocity tail [13] that is responsible for the divergence of high-degree moments [9,12]. It is then possible that the entropy does not capture the rather rich structure of the Boltzmann distribution function for high velocities and remains dominated by the population of thermal velocities, which is less "ordered" than in the case of the BGK distribution.
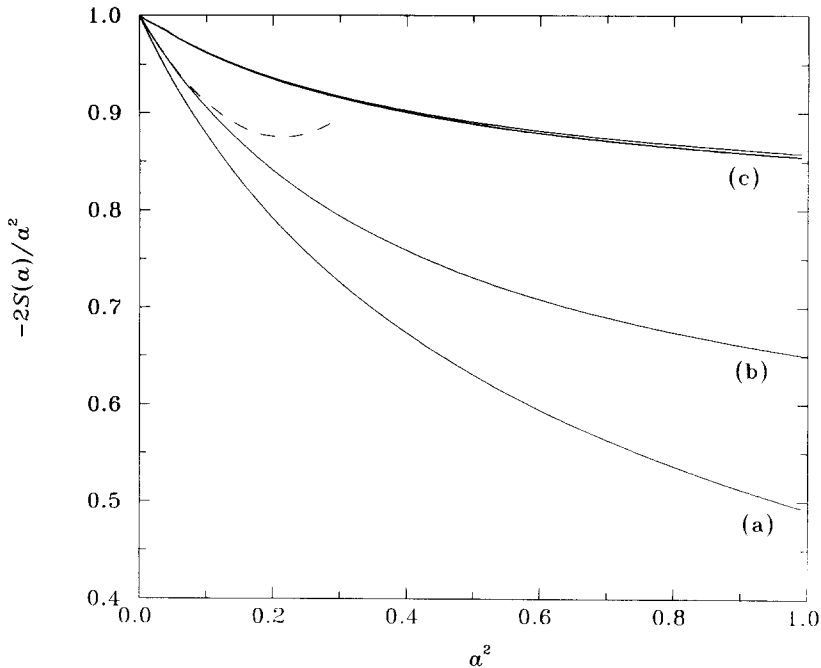
Fig. 2. Plot of $-2S(a)/a^2$ versus a^2 according to (a) information theory, (b) the Padé (1,1) obtained from the Boltzmann equation, and (c) the Padés (2,2) and (3,3) (lower curve) and the Padé (4,4) (upper curve) obtained from the BGK equation. The dashed line corresponds to the truncated power series obtained from the Boltzmann equation.

Acknowledgements

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