

## Does the Gaussian Thermostat Maximize the Phase-Space Compression Factor?

J. M. Montanero,<sup>1</sup> A. Santos,<sup>1</sup> and V. Garzó<sup>1</sup>

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A recent hypothesis of D. J. Evans and A. Baranyai according to which the Gaussian thermostat maximizes the average phase-space compression factor  $\Lambda$  in nonequilibrium steady states is analyzed for a dilute gas under uniform shear flow. Three routes have been followed: (i) an exact solution of the Bhatnagar–Gross–Krook kinetic equation for arbitrary shear rate, (ii) an exact solution of the Boltzmann equation through super-Burnett order, and (iii) a numerical solution of the Boltzmann equation for finite shear rates. The results show that the above hypothesis does not exactly hold for arbitrary shear rates, although the thermostat that maximizes  $\Lambda$  is close to the Gaussian one. In addition, the influence of the thermostat considered on the nonlinear shear viscosity is also analyzed.

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**KEY WORDS:** Phase-space compression factor; thermostat forces; uniform shear flow; Boltzmann equation.

### 1. INTRODUCTION

In nonequilibrium molecular dynamics simulations, deterministic thermostats are usually introduced to remove the heat produced so that nonequilibrium steady states are achieved.<sup>(1,2)</sup> In this context, a thermostat adopts the form of an external force  $\mathcal{F}$  acting on each particle. Gauss' principle of least constraint provides the simplest choice for  $\mathcal{F}$ , namely  $\mathcal{F} = -m\alpha_0 \mathbf{V}$ , where  $\mathbf{V}$  is the peculiar velocity and  $m$  is the mass of a particle.<sup>(1,2)</sup> In general, the presence of the thermostat force implies that the volume of the phase space accessible to the steady state decreases in time. The rate of change of this volume is measured by the phase-space compression factor (which is a negative quantity). Its average  $\Lambda$  is proportional to the time derivative of the Gibbs entropy.<sup>(3)</sup>

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<sup>1</sup> Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain.

Recently, Evans and Baranyai<sup>(4)</sup> have proposed a variational principle to characterize nonequilibrium steady states. This principle states that  $A$  is a local maximum with respect to variations of endogenous variables. Such a hypothesis is a generalization of the principle of minimum entropy production<sup>(5)</sup> to far-from-equilibrium states. In addition, they conjecture that within several wide classes of possible thermostats, the Gaussian thermostat maximizes the phase-space compression factor.<sup>(3)</sup> To support their hypotheses, Evans and Baranyai provided simulation data for a thermostatted dense fluid under uniform shear flow. Other extremum properties of the Gaussian thermostat have also been proposed and tested by computer simulations.<sup>(6)</sup>

Although the above hypotheses seem to be supported by numerical evidence, it is clear that a theoretical analysis is desirable. This requires a study of the properties of the system far from equilibrium. Consequently, it is convenient to consider a tractable system for which a detailed description can be offered. The prototype fluid for the study of nonequilibrium properties is a monatomic low-density gas with short-range interactions. The physical information is given by the one-particle velocity distribution function, which obeys the nonlinear Boltzmann equation.<sup>(7)</sup> Starting from *exact* solutions of the Boltzmann equation<sup>(8)</sup> and of the Bhatnagar–Gross–Krook (BGK) model kinetic equation,<sup>(9)</sup> it has been proved that the Evans–Baranyai variational principle is *not* verified arbitrarily far from equilibrium.

The aim of this paper is twofold. First, we want to investigate whether the Gaussian thermostat maximizes the phase-space compression factor of a dilute gas under uniform shear flow. If this were the case, this would provide a reason, additional to Gauss' principle, to choose the thermostat  $\mathcal{F} = -m\alpha_0 \mathbf{V}$  among different possible thermostats. Second, we are interested in analyzing the influence of the thermostat considered on the main transport property of the system, namely the shear viscosity coefficient. In particular, we will study the extent to which the *nonlinear* shear viscosity is affected by small deviations from the Gaussian thermostat. In order to address the above points, we will follow three complementary routes: (i) an exact solution of the BGK model kinetic equation for arbitrary shear rates, (ii) an exact solution of the nonlinear Boltzmann equation for Maxwell molecules up to third order in the shear rate, and (iii) a numerical solution of the Boltzmann equation by means of the direct simulation Monte Carlo (DSMC) method<sup>(10)</sup> for finite shear rates.

This paper is organized as follows. In Section 2 the problem is posed and the class of thermostats considered is defined. The relevant quantities of the problem are obtained in terms of quantities evaluated with the Gaussian thermostat. The expressions hold for the Boltzmann equation in

the case of Maxwell molecules and for the BGK equation for general interaction potentials. The latter case is worked out in Section 3 by making use of the known solution of the BGK equation for a Gaussian thermostat and arbitrary shear rate.<sup>(11)</sup> The case of the Boltzmann equation is considered in Section 4, where a Chapman–Enskog solution recently derived<sup>(12)</sup> is used. This is complemented with numerical results for finite shear rates. Finally, the results are discussed in Section 5.

## 2. DESCRIPTION OF THE PROBLEM

As an adequate example of nonequilibrium steady state, let us consider the uniform shear flow, namely a state with a constant density and temperature and a linear velocity profile of the form  $u_x = ay$ ,  $a$  being the constant shear rate. To achieve a steady state, a thermostat external force  $\mathcal{F}$  is introduced. We choose the following class of thermostats ( $\mu$ -thermostats):

$$\mathcal{F}_i = -m\alpha(|V_i|^\mu V_i - \xi_i), \quad i = x, y, z \quad (1)$$

The thermostat parameter  $\alpha$  is a function of  $\mu$  and  $a$ . The constant  $\xi_i$  is introduced to preserve momentum conservation. When one particularizes to  $\mu = 0$ , then  $\xi_i = 0$  and Eq. (1) reduces to the Gaussian thermostat. The uniform shear flow state and the  $\mu$ -thermostats have been considered by Evans and co-workers<sup>(3,6)</sup> to test the extremum properties of the Gaussian thermostat by computer simulations. In this paper, we analyze the problem by taking the Boltzmann equation as a starting point. Under the above conditions, the Boltzmann equation reads<sup>(13)</sup>

$$-aV_y \frac{\partial}{\partial V_x} f - \alpha \frac{\partial}{\partial V_i} (V_i |V_i|^\mu - \xi_i) f = J[f, f] \quad (2)$$

where  $J[f, f]$  is the nonlinear Boltzmann collision operator<sup>(7)</sup> and  $f(\mathbf{V})$  is the one-particle velocity distribution function. Conservation of momentum ( $\langle \mathbf{V} \rangle = 0$ ) implies that  $\xi_i = \langle V_i |V_i|^\mu \rangle$ , where

$$\langle A(\mathbf{V}) \rangle = \frac{1}{n} \int d\mathbf{V} A(\mathbf{V}) f(\mathbf{V}) \quad (3)$$

$n$  is the number density. The average phase-space compression factor corresponding to  $\mu$ -thermostats is obtained in ref. 3. In the context of a dilute gas, it becomes

$$A = -\alpha(\mu + 1) \langle |V_x|^\mu + |V_y|^\mu + |V_z|^\mu \rangle \quad (4)$$

According to the hypothesis proposed by Evans and Baranyai,<sup>(3)</sup>  $A$  is a maximum at  $\mu = 0$  for arbitrary shear rates. Consequently,  $\lambda = 0$ , where

$$\lambda \equiv \frac{1}{A} \frac{\partial A}{\partial \mu} \Big|_{\mu=0} \tag{5}$$

Our main goal is to evaluate  $\lambda(a)$  from Eq. (2). To this end, we expand  $f$  and  $\alpha$  in powers of  $\mu$ :

$$f = f_0 + \mu f_1 + \dots \tag{6}$$

$$\alpha = \alpha_0 + \mu \alpha_1 + \dots \tag{7}$$

where the shear rate  $a$  is kept fixed. Analogously,

$$A = A_0 [1 + \mu \lambda + \dots] \tag{8}$$

Insertion of these expansions into Eq. (2) yields

$$-a V_y \frac{\partial}{\partial V_x} f_0 - \alpha_0 \frac{\partial}{\partial V_i} V_i f_0 = J[f_0, f_0] \tag{9}$$

$$\begin{aligned} -a V_y \frac{\partial}{\partial V_x} f_1 - \frac{\partial}{\partial V_i} [V_i (\alpha_0 f_1 + \alpha_1 f_0 + \alpha_0 \log |V_i| f_0) \\ - \alpha_0 \langle V_i \log |V_i| \rangle_0 f_0] = J[f_0, f_1] + J[f_1, f_0] \end{aligned} \tag{10}$$

The knowledge of  $f$  and  $\alpha$  up to first order in  $\mu$  is sufficient to determine  $\lambda$ . It is given as

$$\lambda = 1 + \frac{\alpha_1}{\alpha_0} + \frac{1}{3} \langle \log |V_x| + \log |V_y| + \log |V_z| \rangle_0 \tag{11}$$

where  $\langle A(\mathbf{V}) \rangle_k$  is evaluated with the distribution  $f_k$ . The coefficient  $\alpha_1$  is determined from the consistency condition

$$\langle V_x^2 + V_y^2 + V_z^2 \rangle_1 = 0 \tag{12}$$

Apart from obtaining  $\lambda$ , it is also interesting to analyze the influence of the choice of the thermostat on the nonlinear shear viscosity

$$\eta = - \frac{P_{xy}}{a} \tag{13}$$

where  $P_{ij} = mn \langle V_i V_j \rangle$  is the pressure tensor. In particular, we want to calculate the quantity

$$\Theta \equiv \frac{1}{\eta} \frac{\partial \eta}{\partial \mu} \Big|_{\mu=0} \quad (14)$$

so that

$$\eta = \eta_0 [1 + \mu \Theta + \dots] \quad (15)$$

Equation (9) describes the uniform shear flow state in the presence of a Gaussian thermostat. Its solution is necessary to solve Eq. (10) and to get the relevant parameters of the problem. Equation (9) has been studied by the moment method up to fourth degree in the special case of Maxwell molecules (repulsive potential of the form  $r^{-4}$ ).<sup>(14,15)</sup> In particular, one has

$$\alpha_0 = \frac{2}{3} \sinh^2 \left[ \frac{1}{6} \cosh^{-1}(1 + 9a^2) \right] \quad (16)$$

$$\langle V_x^2 \rangle_0 = \frac{1}{2} \frac{1 + 6\alpha_0}{1 + 2\alpha_0} \quad (17)$$

$$\langle V_y^2 \rangle_0 = \langle V_z^2 \rangle_0 = \frac{1}{2} \frac{1}{1 + 2\alpha_0} \quad (18)$$

$$\langle V_x V_y \rangle_0 = -\frac{1}{2} \frac{a}{(1 + 2\alpha_0)^2} \quad (19)$$

In these equations, we have chosen units such that  $2k_B T/m = 1$ , where  $T$  is the temperature, and  $\zeta = 1$ ,  $\zeta$  being a convenient effective collision frequency.

It must be noticed that the *exact* knowledge of a *finite* number of moments of  $f_0$  is not sufficient to get averages such as  $\langle \log |V_i| \rangle_0$ . Consequently, one needs to know the explicit expression of  $f_0$ . This function has been recently derived through super-Burnett order ( $a^3$ ).<sup>(12)</sup> Another possibility is to use the solution of Eq. (9) when  $J[f_0, f_0]$  is replaced by the BGK collision term.<sup>(16)</sup> This solution has been derived in ref. 11 and applies for general interaction potentials and arbitrary shear rates.

In the remainder of this section we will express the quantities  $\alpha_1$ ,  $\lambda$ , and  $\Theta$  in terms of averages with  $f_0$ . Here, we will assume that the particles interact through the Maxwell potential. Multiplying both sides of Eq. (10) by  $V_i V_j$  and integrating over  $\mathbf{V}$ , one gets

$$\begin{aligned} a(\delta_{ix} \langle V_j V_y \rangle_1 + \delta_{jx} \langle V_i V_y \rangle_1) + 2\alpha_0 \langle V_i V_j \rangle_1 + 2\alpha_1 \langle V_i V_j \rangle_0 \\ + \alpha_0 \langle V_i V_j (\log |V_i| + \log |V_j|) \rangle_0 = -\langle V_i V_j \rangle_1 \end{aligned} \quad (20)$$

This equation gives  $\langle V_i V_j \rangle_1$  in terms of  $\alpha_1$  and  $\langle \dots \rangle_0$ . Condition (12) provides the expression of  $\alpha_1$ :

$$\alpha_1 = \frac{2}{3} \alpha_0 \frac{1 + 2\alpha_0}{1 + 6\alpha_0} \left[ 3\alpha_0(1 + 2\alpha_0) \frac{1}{a} \langle V_x V_y (\log |V_x| + \log |V_y|) \rangle_0 \right. \\ \left. - \langle V_x^2 \log |V_x| \rangle_0 - (1 + 6\alpha_0) \langle V_y^2 \log |V_y| \rangle_0 - \langle V_z^2 \log |V_z| \rangle_0 \right] \quad (21)$$

where use has been made of Eqs. (16)–(19). The expression of  $\lambda$  follows from Eqs. (11) and (21). Furthermore, the expression of  $\Theta = \langle V_x V_y \rangle_1 / \langle V_x V_y \rangle_0$  is

$$\Theta = \alpha_0(1 + 2\alpha_0) \frac{1}{a} \langle V_x V_y (\log |V_x| + \log |V_y|) \rangle_0 \\ - 2\alpha_0 \langle V_y^2 \log |V_y| \rangle_0 - \frac{2\alpha_1}{1 + 2\alpha_0} \quad (22)$$

The leading behaviors of  $\lambda$  and  $\Theta$  for small shear rates will be exactly obtained in Section 4 in the case of the Boltzmann equation for Maxwell molecules. Before that, the general shear-rate dependence of these quantities will be derived in Section 3 from the BGK kinetic model.

### 3. RESULTS FROM THE BGK EQUATION

The BGK collision term is defined as<sup>(16)</sup>

$$J[f, f] \rightarrow -\zeta(f - f^{\text{LE}}) \quad (23)$$

where  $\zeta$  is an effective collision frequency and  $f^{\text{LE}}$  is the local equilibrium distribution function. In reduced units, it reads

$$f^{\text{LE}} = n\pi^{-3/2} e^{-V^2} \quad (24)$$

The influence of the interaction potential is modeled through the temperature dependence of  $\zeta$ . In the thermostatted uniform shear flow state,  $\zeta$  is a constant, so that the results are independent of the interaction considered when one takes  $\zeta^{-1} = 1$  as the time unit. The exact solution of Eq. (9) with the replacement (23) is given by<sup>(11)</sup>

$$f_0(\mathbf{V}) = \pi^{-3/2} \int_0^\infty ds \exp[-(1 - 3\alpha_0)s] \exp\left(asV_y \frac{\partial}{\partial V_x}\right) \exp(-e^{2\alpha_0 s} V^2) \quad (25)$$

Here,  $\alpha_0$  is also given by Eq. (16). The action of the operator in Eq. (25) is

$$\exp\left(asV_y \frac{\partial}{\partial V_x}\right) \Psi(V_x, V_y, V_z) = \Psi(V_x + asV_y, V_y, V_z) \quad (26)$$

From Eq. (25) one can get the velocity moments. In particular, the second-degree moments coincide with those of the Boltzmann equation for Maxwell molecules, Eqs. (17)–(19). Moments of higher degree are different in both equations.<sup>(17)</sup>

The explicit knowledge of  $f_0$  allows us to evaluate analytically the averages appearing in the expressions for  $\lambda$ , Eq. (11),  $\alpha_1$ , Eq. (21), and  $\Theta$ , Eq. (22). Those averages are calculated in Appendix A. Putting together all the results, one finally arrives at

$$\alpha_1 = -\alpha_0 \left[ 4A^{(2)} + \frac{\Phi^{(0)}(3\alpha_0)}{6(1+6\alpha_0)} + \frac{\alpha_0}{2} \frac{\Phi^{(1)}(3\alpha_0) + \Phi^{(2)}(3\alpha_0)}{1+6\alpha_0} - \alpha_0 \frac{1+12\alpha_0}{(1+2\alpha_0)(1+6\alpha_0)} \right] \quad (27)$$

$$\lambda = 1 + \frac{\alpha_1}{\alpha_0} + 2A^{(0)} - \alpha_0 + \frac{1}{6} \Phi^{(0)}(a^2) \quad (28)$$

$$\Theta = -\frac{\alpha_0}{1+6\alpha_0} \left[ -\frac{4}{3} \frac{\Phi^{(0)}(3\alpha_0)}{1+2\alpha_0} + \Phi^{(1)}(3\alpha_0) - \frac{4\alpha_0}{1+2\alpha_0} \Phi^{(2)}(3\alpha_0) - 4\alpha_0 \frac{1-6\alpha_0}{(1+2\alpha_0)^2} \right] \quad (29)$$

In these equations, we have introduced the constants

$$A^{(n)} \equiv \pi^{-1/2} \int_0^\infty dx x^n \log x e^{-x^2} \quad (30)$$

and the functions

$$\Phi^{(n)} \equiv \int_0^\infty ds e^{-s} s^n \log(1+xs^2) \quad (31)$$

Some properties of  $A^{(n)}$  and  $\Phi^{(n)}$  are given in Appendix B.

It is quite evident that  $\lambda \neq 0$  for arbitrary shear rates. This means that, in the context of the BGK equation, the phase-space compression factor is

not maximum for the Gaussian thermostat. For small shear rates, one has

$$\alpha_1 = -\frac{4}{3}A^{(2)}a^2 + \frac{16}{9}A^{(2)}a^4 - \frac{17 + 112A^{(2)}}{27}a^6 + \mathcal{O}(a^8) \quad (32)$$

$$\lambda = -\frac{31}{9}a^4 + \mathcal{O}(a^6) \quad (33)$$

$$\Theta = -\frac{1}{3}a^4 + \mathcal{O}(a^6) \quad (34)$$

The fact that  $\lambda$  is of order  $a^4$  in the BGK model means that the Evans–Baranyai hypothesis can be considered as a good approximation for small shear rates. Similarly, according to Eq. (34), the shear viscosity up to super-Burnett order is not affected by slight variations of the thermostat with respect to the Gaussian one.

#### 4. RESULTS FROM THE BOLTZMANN EQUATION

As said in Section 2, the knowledge of  $f_0$  (or, equivalently, of the infinite set of its velocity moments) is required to evaluate the averages appearing in the expressions for  $\alpha_1$ ,  $\lambda$ , and  $\Theta$ . Even though Eq. (9) can be, in principle, recursively solved by the moment method for Maxwell molecules, this method does not seem to be of practical use for evaluating averages such as  $\langle \log |V_i| \rangle_0$ . As a consequence, we restrict ourselves to the domain of small shear rates, for which a Chapman–Enskog expansion is adequate.<sup>(7,16)</sup> In order to obtain the leading behaviors of  $\lambda$  and  $\Theta$ , it is necessary to know  $f_0$  through order  $a^3$ . Such an expansion has been performed in ref. 12. From it, one can easily get

$$\langle \log |V_x| \rangle_0 = 2A^{(0)} + \left( \frac{467}{1470} + \frac{16}{35\gamma} \right) a^2 + \mathcal{O}(a^4) \quad (35)$$

$$\langle \log |V_y| \rangle_0 = 2A^{(0)} + \left( -\frac{1003}{1470} + \frac{16}{35\gamma} \right) a^2 + \mathcal{O}(a^4) \quad (36)$$

$$\langle \log |V_z| \rangle_0 = 2A^{(0)} - \left( \frac{493}{1470} + \frac{4}{35\gamma} \right) a^2 + \mathcal{O}(a^4) \quad (37)$$

$$\langle V_x^2 \log |V_x| \rangle_0 = 2A^{(2)} + \left( \frac{1493}{2940} + \frac{8A^{(2)}}{3} - \frac{8}{35\gamma} \right) a^2 + \mathcal{O}(a^4) \quad (38)$$

$$\langle V_y^2 \log |V_y| \rangle_0 = 2A^{(2)} + \left( \frac{23}{2940} - \frac{4A^{(2)}}{3} - \frac{8}{35\gamma} \right) a^2 + \mathcal{O}(a^4) \quad (39)$$

$$\langle V_z^2 \log |V_z| \rangle_0 = 2A^{(2)} + \left( \frac{-487}{2940} - \frac{4A^{(2)}}{3} + \frac{2}{35\gamma} \right) a^2 + \mathcal{O}(a^4) \quad (40)$$



$$\begin{aligned}
 & \frac{1}{a} \langle V_x V_y \log |V_y| \rangle_0 \\
 &= -2A^{(2)} + \frac{1}{1584660\gamma^2\gamma'(49 + 24\gamma)(-49 + 69\gamma)} \\
 & \quad \times \{ -3416526960\gamma' + (-5534208960 + 1064012754\gamma')\gamma \\
 & \quad + [12000198000 + (5342978669 - 10146049760A^{(2)}\gamma')\gamma^2 \\
 & \quad + [-3919584480 + (942088581 + 9317800800A^{(2)}\gamma')\gamma^3 \\
 & \quad + [-3500658000 + (-937477224 + 6997858560A^{(2)}\gamma')\gamma^4 \\
 & \quad + 954253440\gamma^5] a^2 + \mathcal{O}(a^4) \tag{41}
 \end{aligned}$$

$$\frac{1}{a} \langle V_x V_y \log |V_x| \rangle_0 = \frac{1}{a} \langle V_x V_y \log |V_y| \rangle_0 - \frac{4 + 2\gamma - \gamma^2}{2\gamma^2} a^2 + \mathcal{O}(a^4) \tag{42}$$

where  $\simeq 1.8731$  and  $\gamma' \simeq 2.4532$  are ratios of eigenvalues of the linearized collision operator. Insertion of the expansions (35)–(42) into Eqs. (11), (21), and (22) yields

$$\alpha_1 = -\frac{4}{3} A^{(2)} a^2 + \left[ \frac{16}{9} A^{(2)} - \frac{7\gamma - 8}{90\gamma} \right] a^4 + \mathcal{O}(a^6) \tag{43}$$

$$\lambda = -\frac{7\gamma - 8}{15\gamma} a^2 + \mathcal{O}(a^4) \tag{44}$$

$$\Theta = Ca^4 + \mathcal{O}(a^6) \tag{45}$$

where  $C$  is a coefficient that can be expressed in terms of  $\gamma$  and  $\gamma'$  and whose numerical value is  $C \simeq 0.05588$ . Equation (44) shows again that  $\lambda \neq 0$  for  $a \neq 0$ . In addition,  $\lambda$  is of order  $a^2$ , in contrast to what happens in the BGK model, Eq. (33). This qualitative discrepancy is related to symmetry properties of the BGK model, which are not present in the Boltzmann equation. For instance,  $\langle \log |V_y| \rangle_0 = \langle \log |V_z| \rangle_0$  and  $\langle V_y^2 \log |V_y| \rangle_0 = \langle V_z^2 \log |V_z| \rangle_0$  in the BGK equation, while these equivalences do not hold in the Boltzmann equation, even at the Burnett order. Similar conclusions with respect to the Evans–Baranyai variational principle<sup>(4)</sup> have been recently found in comparing the predictions of the Boltzmann and BGK equations.<sup>(8)</sup>

In order to study the behavior of  $\lambda$  and  $\Theta$  for finite shear rates, we have numerically solved Eq. (9) by means of the direct simulation Monte

Carlo (DSMC) method.<sup>(10)</sup> We have considered the shear rates  $a=0.1, 0.2, \dots, 1.0$ , and have evaluated the averages needed for the calculations of the relevant quantities. Figure 1 shows the shear-rate dependence of  $\lambda$ . The solid line represents the BGK results, Eqs. (28) and (29), while the dots are the simulation results. It is interesting to point out that both the BGK and the Boltzmann equations predict that the magnitude of  $\lambda$  increases as the shear rate increases. On the other hand, the BGK equation underestimates the absolute value of  $\lambda$ . As a matter of fact, for small shear rates,  $\lambda \sim a^4$  in the BGK model, while  $\lambda \sim a^2$  in the Boltzmann equation. The fact that  $\lambda$  is negative means, according to Eq. (8), that the phase-space compression factor  $\mathcal{A}$  increases (i.e., its absolute value decreases) as  $\mu$  increases around  $\mu=0$ . Anyway, the numerical value of  $\lambda$  in the region considered in Fig. 1 is sufficiently small to speculate that the value of  $\mu$  that maximizes  $\mathcal{A}$  is relatively close to  $\mu=0$ .

In Fig. 2 we plot  $\Theta$  versus  $a^2$ . Now the discrepancy between the BGK and the Boltzmann values is less remarkable than in the case of  $\lambda$ . Besides, the BGK equation overestimates the influence of the choice of a non-Gaussian thermostat. In any case, this influence is not quite important. Equation (15) allows one to estimate that, for instance, the shear viscosity at  $a=1$  (for which the shear viscosity is about one-half the Navier–Stokes value) and  $\mu=0.1$  has increased about 0.4% with respect to the value corresponding to the Gaussian thermostat.

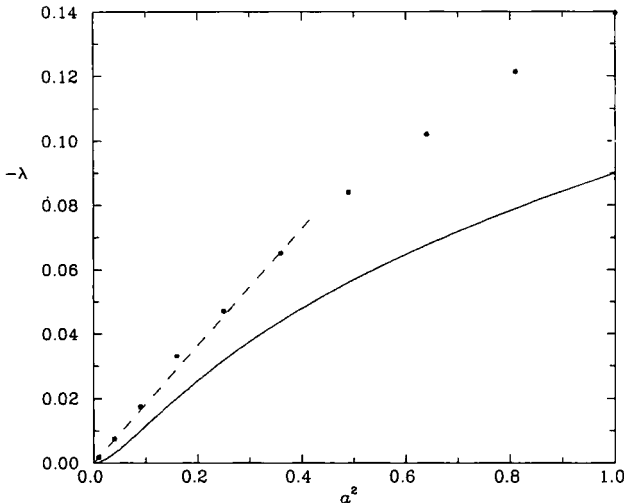


Fig. 1. Shear-rate dependence of  $\lambda$ . The solid line refers to the BGK results, while the dots represent the simulation results for the Boltzmann equation. The dashed line is the exact leading behavior for small shear rates.

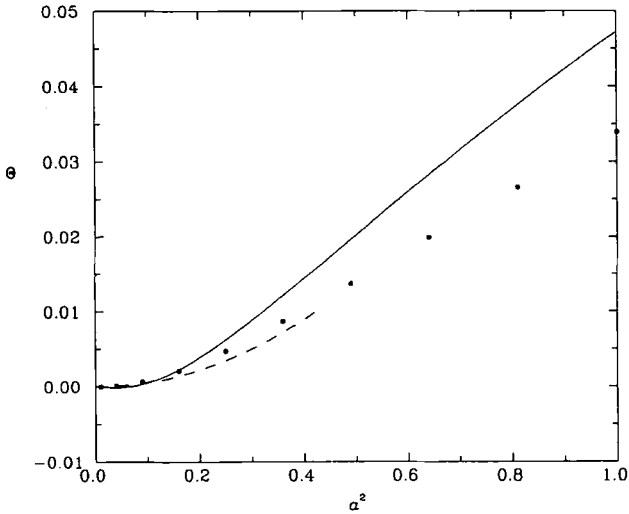


Fig. 2. The same as in Fig. 1, but for  $\Theta$ .

## 5. CONCLUSIONS

Nonconservative thermostat forces are commonly used in non-equilibrium molecular dynamics to simulate steady states far from equilibrium. A consequence of the presence of thermostats is that the phase-space volume accessible to the steady state decreases in time. In principle, for a given state, the transport properties, as well as the phase-space compression factor, can be affected by the choice of the thermostat force. Gauss' principle of least constraint gives a mechanical criterion to select the force:  $\mathcal{F} = -m\alpha_0 \mathbf{V}$ . Furthermore, it has been recently conjectured that the Gaussian thermostat presents some extremum properties.<sup>(3,6)</sup> In particular, it maximizes the average phase-space compression factor  $\Lambda$ . No theoretical proof of this hypothesis exists, although it is supported by computer simulations of dense fluids under uniform shear flow.

In this paper, we have tested the validity of the above hypothesis and measured the influence of non-Gaussian thermostats on the transport coefficient, namely the nonlinear shear viscosity  $\eta$ , in a dilute gas under uniform shear flow. As in ref. 6, we have considered the family of the so-called  $\mu$ -thermostats, i.e.,  $\mathcal{F}_i = -m\alpha(|V_i|^\mu V_i - \xi_i)$ . We have addressed our attention to the coefficients  $\lambda$  and  $\Theta$ , which are related to the first derivatives of  $\Lambda$  and  $\eta$ , respectively, with respect to  $\mu$  at  $\mu=0$ . By starting from the Boltzmann equation for Maxwell molecules, we have expressed  $\lambda$

and  $\Theta$  in terms of quantities defined with the Gaussian thermostat and for arbitrary shear rate  $a$ . These expressions also hold for the BGK kinetic model and general interaction potentials.

From the explicit solution of the BGK equation in the case of the Gaussian thermostat, we have obtained the shear rate dependence of  $\lambda$  and  $\Theta$ . A similar calculation cannot be made in the case of the Boltzmann equation, since its exact solution is not known for arbitrary  $a$ . On the other hand, we have taken advantage of the knowledge of the distribution function through third order in  $a$  to evaluate the leading behavior of  $\lambda$  and  $\Theta$ . This information is complemented by numerically solving the Boltzmann equation at finite shear rates by means of the DSMC method.<sup>(10)</sup> The results show that  $\lambda \neq 0$ , so that  $\Lambda$  is not a maximum at  $\mu = 0$ , from a strict point of view. Besides, the magnitude of  $\lambda$  increases with the shear rate. Nevertheless, the fact that  $\lambda$  is small, even for shear rate as large as  $a = 1$ , suggests that the value of  $\mu$  that maximizes  $\Lambda$  is close to  $\mu = 0$ . For instance, if  $\mu = 0.1$  and  $a = 1$ , the magnitude of the phase-space compression factor decreases only by about 1%. This could explain why the molecular dynamics results<sup>(3)</sup> showed that  $\Lambda$  is maximum at  $\mu = 0$ , since the closest values to  $\mu = 0$  considered were  $\mu = \pm 0.25$ . In addition, it must be noticed that the simulations were carried out for a two-dimensional dense fluid and the numerical value of  $\lambda$  is expected to depend on the density and dimensionality of the system.

Concerning the coefficient  $\Theta$ , which is related to the dependence of  $\eta$  on  $\mu$ , the results show that it increases with the shear rate. Nevertheless, a small deviation from the Gaussian thermostat has a less noticeable effect on the shear viscosity than on the phase-space compression factor. Consequently, the value of  $\mu$  that maximizes  $\eta$  is possibly closer to  $\mu = 0$  than the one that maximizes  $\Lambda$ . This conclusion is similar to the one obtained in ref. 8 in connection with the Evans–Baranyai variational principle.<sup>(4)</sup>

We think that if the introduction of an artificial thermostat force is needed to “manufacture” a certain nonequilibrium steady state, the only criterion to choose the thermostat is that of simplicity. From that point of view, the Gaussian thermostat is the most appropriate one. Other criteria, such as extremizing some physical quantities, lead in general to different choices, which are also dependent on how far the state is from equilibrium.

It must also be pointed out that one can define a nonlinear shear viscosity in the USF state without any thermostat.<sup>(18)</sup> In general, such a viscosity differs from that of thermostatted systems,<sup>(19)</sup> except for a dilute gas of Maxwell molecules. For instance, the super-Burnett coefficients for a gas of hard spheres differ by about 33%.<sup>(13)</sup>

Finally, it is important to remark that, in contrast to the conclusions of some authors,<sup>(20)</sup> the uniform shear flow state (which is generated in the

computer by means of the so-called Slod algorithm<sup>(1)</sup> or by imposing Lees–Edwards boundary conditions<sup>(21)</sup> leads to a nonlinear shear viscosity different from the one obtained by means of realistic boundary conditions.<sup>(22)</sup> This point has been recently clarified in ref. 23.

## APPENDIX A. CALCULATION OF SOME VELOCITY INTEGRALS FROM THE BGK SOLUTION

In this appendix we evaluate the averages appearing in Eqs. (11), (21), and (22) by using the solution (25) of the BGK equation. In the following, we will make use of the general property

$$\int d\mathbf{V} G(\mathbf{V}) e^{asV_y \partial/\partial V_x} F(\mathbf{V}) = \int d\mathbf{V} F(\mathbf{V}) e^{-asV_y \partial/\partial V_x} G(\mathbf{V}) \quad (\text{A1})$$

Let us first evaluate  $\langle \log |V_y| \rangle_0$ :

$$\begin{aligned} \langle \log |V_y| \rangle_0 &= \pi^{-3/2} \int_0^\infty ds \{ \exp[ -(1 - 3\alpha_0)s ] \} \\ &\quad \times \int d\mathbf{V} \log |V_y| \exp(-e^{2\alpha_0 s} V^2) \\ &= \pi^{-3/2} \int_0^\infty ds e^{-s} \int d\xi [ \log |\xi_y| - \alpha_0 s ] e^{-\xi^2} \\ &= 2\mathcal{A}^{(0)} - \alpha_0 \end{aligned} \quad (\text{A2})$$

where in the second step we have made the change  $\xi = e^{\alpha_0 s} \mathbf{V}$  and in the last step we have used the definition (30). By following similar steps, one finds

$$\langle \log |V_z| \rangle_0 = \langle \log |V_y| \rangle_0 \quad (\text{A3})$$

$$\begin{aligned} \langle V_y^2 \log |V_y| \rangle_0 &= \langle V_z^2 \log |V_z| \rangle_0 \\ &= \frac{1}{1 + 2\alpha_0} \left[ 2\mathcal{A}^{(2)} - \frac{1}{2} \frac{\alpha_0}{1 + 2\alpha_0} \right] \end{aligned} \quad (\text{A4})$$

$$\langle V_x V_y \log |V_y| \rangle_0 = -\frac{a}{(1 + 2\alpha_0)^2} \left[ 2\mathcal{A}^{(2)} - \frac{\alpha_0}{1 + 2\alpha_0} \right] \quad (\text{A5})$$

Next, we evaluate  $\langle \log |V_x| \rangle_0$ :

$$\begin{aligned} \langle \log |V_x| \rangle_0 &= \pi^{-3/2} \int_0^\infty ds \{ \exp[ -(1 - 3\alpha_0)s ] \} \\ &\quad \times \int d\mathbf{V} \log |V_x - asV_y| \exp(-e^{2\alpha_0 s} V^2) \\ &= \pi^{-3/2} \int_0^\infty ds e^{-s} \int d\xi [ \log |\xi_x| + \frac{1}{2} \log(1 + a^2 s^2) - \alpha_0 s ] e^{-\xi^2} \\ &= 2A^{(0)} - \alpha_0 + \frac{1}{2} \Phi^{(0)}(a^2) \end{aligned} \tag{A6}$$

Now, in the second step we have made the change

$$\xi = e^{\alpha_0 s} \mathbf{M} \cdot \mathbf{V} \tag{A7}$$

where

$$\mathbf{M} = \frac{1}{(1 + a^2 s^2)^{1/2}} \begin{pmatrix} 1 & -as & 0 \\ as & 1 & 0 \\ 0 & 0 & (1 + a^2 s^2)^{1/2} \end{pmatrix} \tag{A8}$$

In the last step of Eq. (A6) we have taken into account the definition (31). Similarly, one gets

$$\begin{aligned} \langle V_x V_y \log |V_x| \rangle_0 &= -\frac{a}{(1 + 2\alpha_0)^2} \left[ 2A^{(2)} - \frac{\alpha_0}{1 + 2\alpha_0} + \frac{1}{4} \Phi^{(1)}(3\alpha_0) \right] \end{aligned} \tag{A9}$$

$$\begin{aligned} \langle V_x^2 \log |V_x| \rangle_0 &= \frac{1}{1 + 2\alpha_0} \left\{ 2A^{(2)}(1 + 6\alpha_0) - \frac{1}{2} \frac{\alpha_0(1 + 18\alpha_0)}{1 + 2\alpha_0} \right. \\ &\quad \left. + \frac{1}{4} [ \Phi^{(0)}(3\alpha_0) + 3\alpha_0 \Phi^{(2)}(3\alpha_0) ] \right\} \end{aligned} \tag{A10}$$

In Eq. (A.10) we used the relation

$$3\alpha_0(1 + 2\alpha_0)^2 = a^2 \tag{A11}$$

whose real solution is Eq. (16).

**APPENDIX B. SOME PROPERTIES OF  $A^{(n)}$  AND  $\Phi^{(n)}$**

In order to evaluate the constants  $A^{(n)}$  defined in Eq. (30), we start from the identity

$$\int_0^\infty dx x^\nu e^{-x^2} = \frac{1}{2} \Gamma\left(\frac{\nu+1}{2}\right) \tag{B1}$$

Differentiation with respect to  $\nu$  yields

$$\int_0^\infty dx x^\nu \log x e^{-x^2} = \frac{1}{4} \Gamma\left(\frac{\nu+1}{2}\right) \Psi\left(\frac{\nu+1}{2}\right) \tag{B1}$$

where  $\Psi(x)$  is the digamma function.<sup>(24)</sup> If we specialize to  $\nu = n = \text{even}$ , we have

$$A^{(n)} = \frac{(n-1)!!}{2^{n/2+2}} \left[ -\gamma_E - 2 \log 2 + 2 \left( 1 + \frac{1}{3} + \dots + \frac{1}{n-1} \right) \right] \tag{B3}$$

where  $\gamma_E = 0.57721 \dots$  is Euler’s constant.

Now, we are going to obtain a representation of the functions  $\Phi^{(n)}(x)$  defined in Eq. (31). First, integration by parts yields

$$\Phi^{(n)}(x) = \int_0^\infty ds e^{-s} \left[ ns^{n-1} \log(1 + xs^2) + 2x \frac{s^{n+1}}{1 + xs^2} \right] \tag{B4}$$

From this equation it is easy to prove the following recurrence relation:

$$\Phi^{(n+1)}(x) = 2x^{-(n-1)/2} \frac{d}{dx} [x^{(n+1)/2} \Phi^{(n)}(x)] \tag{B5}$$

Now, we focus on  $\Phi^{(0)}(x)$ . It can be expressed as<sup>(25)</sup>

$$\Phi^{(0)}(x) = -2[\text{ci}(x^{-1/2}) \cos(x^{-1/2}) + \text{si}(x^{-1/2}) \sin(x^{-1/2})] \tag{B6}$$

where  $\text{si}(z)$  and  $\text{ci}(z)$  are the sine and cosine integrals, respectively. From Eq. (B5) one finds

$$\begin{aligned} \Phi^{(1)}(x) &= \Phi^{(0)}(x) + 2 \\ &+ \frac{2}{\sqrt{x}} [-\text{ci}(x^{-1/2}) \sin(x^{-1/2}) + \text{si}(x^{-1/2}) \cos(x^{-1/2})] \end{aligned} \tag{B7}$$

$$\Phi^{(2)} = 2\Phi^{(1)}(x) + 2 - \frac{1}{x} \Phi^{(0)}(x) \tag{B8}$$

Finally, from Eq. (31) one gets the asymptotic series in powers of  $x$ :

$$\Phi^{(n)}(x) = \sum_{m=0}^{\infty} (-1)^m \frac{(n+2+2m)!}{m+1} x^{m+1} \quad (\text{B9})$$

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