Thermal conductivity of a dilute gas in a thermostated shear-flow state

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An expression for the thermal-conductivity tensor in a steady uniform shear-flow state is derived. The results are obtained by using the Bhatnagar-Gross-Krook model kinetic equation for dilute gases. This tensor is a highly nonlinear function of the shear rate and its expression is not restricted to any specific interaction model. The dependence on the shear rate is illustrated in the case of repulsive potentials of the form $r^{-\mu}$.

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I. INTRODUCTION

The description of transport processes in states near equilibrium is well established. For such situations, the Curie principle shows that when a fluid is subject to a velocity gradient and a temperature gradient, the heat flux is not affected by the presence of the velocity gradient [1]. Nevertheless, when a shear rate is large, nonlinear effects become important and the energy transport is disturbed by the shearing motion.

In the last few years, the uniform shear flow has provided an adequate framework to analyze nonlinear transport properties. In the context of dense gases, Evans [2] has recently derived a generalized Green-Kubo formula for the thermal-conductivity tensor of a shearing fluid. This relation has been extended to the self-diffusion [2] and mutual-diffusion [3] tensors. In addition, several molecular-dynamics simulations have been carried out [3–5] to calculate the shear-rate dependence of the above quantities. All these results refer to situations in which the system is in a thermostatted steady state. On the other hand, some related problems have been studied in the low density limit. For instance, an expression for the shear-rate-dependent self-diffusion tensor has been obtained in the case of mechanically identical Maxwell molecules [6]. Similar studies have been performed to extend the previous problem to the case of binary mixtures in the tracer limit [7]. However, to our knowledge no explicit derivation for the thermal-conductivity tensor in a dilute gas under steady shear flow has been made.

The aim of this paper is to analyze the transport properties in a dilute gas under steady uniform shear flow and subject to a weak thermal gradient. The system is sheared by applying Lees-Edwards periodic boundary conditions [8], so that the velocity profile is linear and the density and the temperature are homogeneous . This type of boundary condition does not preserve conservation of energy since the temperature monotonically increases with time (viscous heating). For this reason, artificial forces must be introduced to achieve a stationary situation. Here, to parallel the analysis made in Ref. [2], we will adopt this point of view. It is clear that this idealized state is desirable for practical purposes, especially in computer simulations.

Preliminary results describing heat transport in a dilute gas under shear flow have been published elsewhere. In the context of the uniform shear flow and in the absence of any external force, an explicit expression for the heat flux in a gas subject to a weak temperature gradient has been derived [9]. This result has been obtained from the Bhatnagar-Gross-Krook (BGK) kinetic equation in the particular case of Maxwell molecules. In this situation the shear flow is disturbed by the presence of the temperature gradient, and consequently a pressure gradient appears in the system. On the other hand, heat transport in the so-called steady Couette flow [10] has also been studied. The physical situation is that of a gas in a stationary state with velocity and temperature gradients. Since the system is sheared by more realistic conditions, the density, the temperature, and the shear rate are nonhomogeneous. Quite surprisingly, although the solution applies for arbitrary velocity and temperature gradients, the heat flux is simply proportional to the temperature gradient (generalized Fourier's law).

Here, we are interested in evaluating the thermal-conductivity tensor in a thermostatted shear-flow state. The main motivation of this work is to present a kinetic theory description to the problem studied by Evans [2] for dense gases. Due to the mathematical difficulties embodied in the Boltzmann equation, we use again the BGK model. In contrast to what occurs in the nonstationary shear flow state [9], the heat flux obeys a generalized Fourier's law where a thermal-conductivity tensor can be identified. It is a highly nonlinear function of the shear rate. Further, it is a nonuniversal function of the shear rate since it depends on the potential model.

In Sec. II we analyze energy transport in a system under steady uniform shear flow. Using a perturbation expansion around the shear-flow state, all the velocity moments up to first order in the thermal gradient are computed. In particular, due to the anisotropy of the system, a thermal-conductivity tensor rather than a scalar is identified. The results are discussed and connected with previous work in Sec. III.

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II. THERMAL-CONDUCTIVITY TENSOR

Let us consider a dilute gas in a steady uniform shear-flow state. At a macroscopic level, this nonequilibrium state is characterized by constant density n and temperature T and a velocity field given by $u_i = a_{ij}r_j$, where $a_{ij} = a\delta_{ix}\delta_{jy}$, a being the constant shear rate. The shearing motion produces viscous heating, so that the temperature increases in time. This problem has motivated the introduction of an (artificial) external force to remove this heating effect. The simplest possibility seems to be a homogeneous nonconservative force proportional to the peculiar velocity $\mathbf{V} = \mathbf{v} - \mathbf{u}$, i.e.,

$$\mathcal{F} = -m\zeta\mathbf{V} , \tag{1}$$

where the thermostat parameter ζ is determined from the condition that the temperature remains constant. It is interesting to consider this situation since most computer simulations include such a thermostat. The uniform shear flow has been extensively studied theoretically [11] and also by means of molecular-dynamics simulations [8].

In a dilute gas, the evolution equation for the velocity distribution function $f(\mathbf{r}, \mathbf{v})$ is the Boltzmann equation. However, the only exact results derived from this equation in the uniform shear flow are restricted to the Maxwell interaction. For other interaction models, one must perform computer simulations. Since we are interested in obtaining an explicit expression for the heat flux valid not only for Maxwell molecules, we consider instead the Bhatnagar-Gross-Krook kinetic equation [11] as a model of the Boltzmann equation. In the case of uniform shear flow, the BGK results exhibit an extremely good agreement with Monte Carlo simulations of the Boltzmann equation [12]. In the BGK model all the details of the interaction potential are introduced through an effective collision frequency ν. It depends on position and time through the local density and temperature. Thus, for repulsive potentials of the form $r^{-\mu}$, $\nu \propto nT^{\alpha}$, with $\alpha = \frac{1}{2} - \frac{2}{\mu}$. Consequently, ν is a constant in the case of steady shear flow. This simplification allows one to evaluate the velocity moments M_{k_1,k_2,k_3} of $f(\mathbf{V})$ in terms of the reduced shear rate $a^* \equiv a/\nu$. They are defined by

$$M_{k_1,k_2,k_3} = \int d\boldsymbol{\xi}\, \xi_x^{k_1}\, \xi_y^{k_2}\, \xi_z^{k_3}\, g(\boldsymbol{\xi}) , \tag{2}$$

where $\boldsymbol{\xi} \equiv (m/2k_BT)^{1/2}\mathbf{V}$ and $g \equiv \frac{1}{n}(2k_BT/m)^{3/2}f$. The only nonvanishing moments correspond to $k_1 + k_2$ and k_3 even, in which case one gets [13]

$$M_{k_1,k_2,k_3} = \pi^{-3/2} \sum_{\substack{q=0 \\ (q+k_1=\text{even})}}^{k_1} (-a^*)^q [1 + \zeta^*(k_1 + k_2 + k_3)]^{-(q+1)} \frac{k_1!}{(k_1 - q)!} \times \Gamma\left(\frac{k_1 - q + 1}{2}\right) \Gamma\left(\frac{k_2 + q + 1}{2}\right) \Gamma\left(\frac{k_3 + 1}{2}\right) , \tag{3}$$

with $\zeta^* \equiv \zeta/\nu$. This parameter can be determined from the consistency condition $M_{200} + M_{020} + M_{002} = \frac{3}{2}$, that yields a cubic equation whose real root is

$$\zeta^* = \tfrac{2}{3} \sinh^2[\tfrac{1}{6} \cosh^{-1}(1 + 9a^{*2})] . \tag{4}$$

We assume now that we perturb the steady shear-flow state by introducing a weak thermal gradient. The presence of a thermal gradient induces the existence of a density gradient, and consequently both the temperature and density are not uniform. Here, we shall assume that the pressure $p = nk_BT$ is constant. For this problem, the BGK equation reads

$$\frac{\partial}{\partial t}f - a_{ij}V_j\frac{\partial}{\partial V_i}f + (V_i + a_{ij}r_j)\frac{\partial}{\partial r_i}f + \frac{\partial}{\partial V_i}\left(\frac{F_i}{m}f\right) = -\nu(f - f^{\text{LE}}) , \tag{5}$$

where f^{LE} is the local equilibrium distribution function defined as

$$f^{\text{LE}} = n\left(\frac{m}{2\pi k_BT}\right)^{3/2} \exp\left(-\frac{m}{2k_BT}V^2\right) . \tag{6}$$

Under the above conditions, one expects that the relevant fluxes are now nonhomogeneous. As a consequence, the linear velocity field can be perturbed by the thermal gradient according to the macroscopic equation for momentum flow. Since we are interested in studying heat transport in a steady state, now it will be necessary to introduce additional external forces. Obviously, in the absence of a thermal gradient, $\mathbf{F}$ is given by the usual thermostat force defined by Eqs. (1) and (4). This point is an important difference with respect to the analysis presented in Ref. [2], where only the usual thermostat force is included.

In order to solve Eq. (5) we shall use a perturbation expansion around the steady shear flow state by taking the temperature gradient ∇T as the perturbation parameter. The main difference of this perturbation scheme from the conventional perturbation methods (Chapman-Enskog, Hilbert) is that the reference zeroth-order state is the shear flow state (with arbitrary shear rate) and not that of local equilibrium. Therefore we write $f = f^{(0)} + f^{(1)} + f^{(2)} + \cdots$, where the corresponding approximations $f^{(k)}$ are nonlinear functions of the shear rate. The distribution $f^{(0)}$ corresponds to the thermostatted shear flow but introducing the local dependence on $n(\mathbf{r})$, $T(\mathbf{r})$, and $\nu(\mathbf{r})$. Since the distributions f and $f^{(0)}$ have the same five conserved moments, the different approximations $f^{(k)}$ must verify the consistency conditions

$$\int d\mathbf{V}(1,\mathbf{V},V^2)f^{(k)}=0\ , \tag{7}$$

for $k\geq 1$. In this paper we will restrict our calculations to first order in ∇T. In the same way as f, the external force $\mathbf{F}$ must be also expanded in powers of ∇T to preserve stationarity of the state . Thus, up to first order in the thermal gradient, $\mathbf{F}=\mathbf{F}^{(0)}+\mathbf{F}^{(1)}$, with $\mathbf{F}^{(0)}\equiv\boldsymbol{\mathcal{F}}$. The force $\mathbf{F}^{(1)}$ will be obtained from the hydrodynamic balance equations derived at this stage. It is clear that the external constraints must be completely specified in far from equilibrium situations as they do not play a neutral role in the transport properties of the system [11].

Since $f^{(0)}$ verifies the BGK equation in the steady shear-flow state, to first order it is found that $f^{(1)}$ obeys the steady equation

$$-\frac{\partial}{\partial V_i}[\zeta V_i+a_{ij}V_j]f^{(1)}+\nu f^{(1)}$$

$$=-(V_i+a_{ij}r_j)\frac{\partial}{\partial r_i}f^{(0)}-\frac{\partial}{\partial V_i}\left(\frac{F_i^{(1)}}{m}f^{(0)}\right)\ . \tag{8}$$

Some remarks follow from the structure of the balance equations associated with Eq. (8). First, the mass balance reads $\mathbf{u}\cdot\nabla n=0$. Consequently, $\mathbf{u}\cdot\nabla T=0$, i.e., the thermal gradient must be orthogonal to the direction of the flow velocity (x axis). It must be noticed that this restriction is necessary to maintain the system in a steady state. An identical conclusion can be obtained from the energy conservation equation. On the other hand, the momentum balance equation leads to the relation

$$\int d\mathbf{V}F_i^{(1)}f^{(0)}=p\frac{\partial}{\partial r_j}P_{ij}^{*(0)}\ , \tag{9}$$

where

$$P_{ij}^{*(0)}=2\int d\boldsymbol{\xi}\ \xi_i\ \xi_j\ g^{(0)} \tag{10}$$

is the reduced pressure tensor whose nonzero components can be obtained from Eq. (3). According to relation (9), it is clear that many choices are in principle possible for $\mathbf{F}^{(1)}$. The simplest form for $\mathbf{F}^{(1)}$ is a constant independent of velocity :

$$F_i^{(1)}=k_BT\frac{\partial}{\partial r_j}P_{ij}^{*(0)}=k_BT\frac{\partial}{\partial T}P_{ij}^{*(0)}\frac{\partial T}{\partial r_j}\ . \tag{11}$$

Notice that $\mathbf{F}^{(1)}$ depends on the potential through the dependence of a^* on T. Equation (11) reflects the anisotropy induced by the shear flow since $\mathbf{F}^{(1)}$ and ∇T are not parallel. Furthermore, since the form of $\mathbf{F}^{(1)}$ has been suggested from the momentum balance equation, one expects that Eq. (11) gives the adequate external field to maintain the system in a shearing steady state, even in the regime of dense gases. It is obvious that in the latter case, the appropriate expression for $P_{ij}^{*(0)}$ would contain collisional contributions due to intermolecular forces.

From Eq. (8), one gets a hierarchy for the velocity moments $M^{(1)}_{k_1,k_2,k_3}$ corresponding to the reduced distribution $g^{(1)}\equiv\frac{1}{n}(2k_BT/m)^{3/2}f^{(1)}$. After some manipulations, one arrives at

$$a^*k_1M^{(1)}_{k_1-1,k_2+1,k_3}+[1+\zeta^*(k_1+k_2+k_3)]M^{(1)}_{k_1,k_2,k_3}=N_{k_1,k_2,k_3}\ , \tag{12}$$

where

$$N_{k_1,k_2,k_3}=A_{k_1,k_2,k_3}\epsilon_y+B_{k_1,k_2,k_3}\epsilon_z\ , \tag{13}$$

$$A_{k_1,k_2,k_3}=-\left[\frac{1}{2}(k_1+k_2+k_3-1)+T\frac{\partial}{\partial T}\right]M^{(0)}_{k_1,k_2+1,k_3}+T\left[k_1M^{(0)}_{k_1-1,k_2,k_3}\frac{\partial}{\partial T}M^{(0)}_{110}+k_2M^{(0)}_{k_1,k_2-1,k_3}\frac{\partial}{\partial T}M^{(0)}_{020}\right]\ , \tag{14}$$

$$B_{k_1,k_2,k_3}=-\left[\frac{1}{2}(k_1+k_2+k_3-1)+T\frac{\partial}{\partial T}\right]M^{(0)}_{k_1,k_2,k_3+1}+k_3M^{(0)}_{k_1,k_2,k_3-1}T\frac{\partial}{\partial T}M^{(0)}_{002}\ , \tag{15}$$

and we have introduced the reduced thermal gradient $\boldsymbol{\epsilon}\equiv\frac{1}{\nu}(2k_BT/m)^{1/2}\nabla\ln T$. In Eqs. (14) and (15), $M^{(0)}$ is given by Eq. (3) and it is assumed that $M^{(0)}$ is identically zero when any of its indices is negative. The solution to Eq. (12) is

$$M^{(1)}_{k_1,k_2,k_3}=\sum_{q=0}^{k_1}(-a^*)^q\left[1+\zeta^*(k_1+k_2+k_3)\right]^{-(q+1)}\times\frac{k_1!}{(k_1-q)!}N_{k_1-q,k_2+q,k_3}\ . \tag{16}$$

Equation (16) provides an explicit expression for the velocity moments of $f^{(1)}$ in terms of the shear rate and the thermal gradient. It has been derived keeping all the orders in the shear rate. Further, expression (16) is not restricted to any specific interaction model. From Eq. (16), the transport of heat across the system can be evaluated. It is defined by

$$\mathbf{J}^{(1)}=\frac{m}{2}\int d\mathbf{V}\ V^2\ \mathbf{V}\ f^{(1)}\ . \tag{17}$$

After some algebra, it is straightforward to show that the heat flux can be cast into the form of a generalized Fourier's law

$$J_i^{(1)} = -\frac{5}{2}\frac{pk_B}{m\nu}\lambda_{ij}(a^*)\frac{\partial T}{\partial r_j} , \tag{18}$$

where λ_{ij} is the reduced thermal-conductivity tensor, which is a highly nonlinear function of a^*. Its explicit form is very large and hence it will be omitted here. The restriction imposed on the symmetry of $\boldsymbol{\nabla} T$ gives rise to the fact that the only relevant components of the thermal-conductivity tensor are λ_{yy}, λ_{zz}, and λ_{xy}. For $a^* = 0$, $\lambda_{ij} = \delta_{ij}$, thus recovering the usual Navier-Stokes result. Equation (18) represents the major result of this paper, since it gives the thermal-conductivity tensor for a dilute gas under arbitrary shear flow. In order to illustrate the shear-rate dependence of λ_{ij}, specific interaction potentials must be considered. For instance, we analyze the particular case of $r^{-\mu}$ potentials for which $(\partial a^*/\partial T) = (1-\alpha)(a^*/T)$. In this case, for small shear rates the behaviors of the components of the thermal-conductivity tensor are $\lambda_{yy} \approx 1+\frac{1}{15}(5+14\alpha)a^{*2}$, $\lambda_{zz} \approx 1+\frac{1}{15}(2\alpha-19)a^{*2}$, and $\lambda_{xy} \approx \frac{2}{5}(\alpha-8)a^*$. For large shear rates, the asymptotic behaviors are $\lambda_{yy} \sim a^{*-2/3}$, $\lambda_{zz} \sim a^{*-2/3}$, and $\lambda_{xy} \sim a^{*-1/3}$. Figure 1 shows λ_{yy} versus a^* for three values of α : $\alpha = 0$ (Maxwell gas), $\alpha = \frac{1}{2}$ (hard spheres), and $\alpha = 1$. The latter case corresponds to a collision frequency proportional to the (constant) pressure, so that $\mathbf{F}^{(1)} = \mathbf{0}$. Although not associated with any physical interaction model, it can be viewed as representing the so-called very-hard-particle (VHP) interaction [14]. For the VHP model, it is easy to show that the heat flux exactly obeys the generalized Fourier's law (18) for every order in the thermal gradient [9]. Further, it is the interaction model for which only the usual thermostat force is necessary to control the stationarity of the system. According to Fig. 1, we see that the shear-rate dependence of λ_{yy} is quite similar for all the interaction models considered. In the region of small shear rates, it increases as the shear rate increases while for finite shear rates λ_{yy} decreases as a^* increases. Further, for a given value of a^*, λ_{yy} increases as the interaction parameter α increases. The component λ_{zz} is much less sensitive to effects of the potential model. It always decreases as a^* increases. The shear flow induces cross effects in the thermal conduction. Thus, a thermal gradient parallel to the gradient of the flow velocity (y axis) creates a transport of heat along the direction of the flow of the system (x axis). These effects are measured by the off-diagonal component λ_{xy}, whose shape is plotted in Fig. 2. For small shear rates, $-\lambda_{xy}$ has practically the same value for all the interaction models while the influence of α on λ_{xy} becomes more noticeable as a^* increases. In this region, $-\lambda_{xy}$ decreases as α decreases at a given value of a^*.

III. DISCUSSION

In this paper, we have addressed the problem of a dilute gas subject to a weak temperature gradient in a strongly shearing state. The description has been made by using the BGK kinetic model. A perturbation expansion around the steady shear-flow state with arbitrary shear rate was carried out to first order in the temperature gradient. In contrast to analysis performed by Evans [2] for dense gases, an additional external force (absent in the pure shear flow) proportional to the thermal gradient was proposed to maintain the stationarity of the state. In the absence of this extra term, the linear velocity field is perturbed by the temperature gradient. In this approximation, all the velocity moments of the velocity distribution function have been explicitly obtained. The thermal-conductivity tensor λ_{ij} is a highly nonlinear function of the shear rate. In addition, it depends on the potential model. There is a particular case for which our description is exact. That corresponds to the VHP interaction model, in which case only the thermostat force, Eq. (1), must be included to achieve a steady state. For this model, the uniform shear flow coexists with a constant temperature gradient for arbitrary values of both the shear rate and the thermal gradient. Although the system is far away from equilibrium, the heat flux is linear with the thermal gradient.

It is interesting to contrast the results presented here

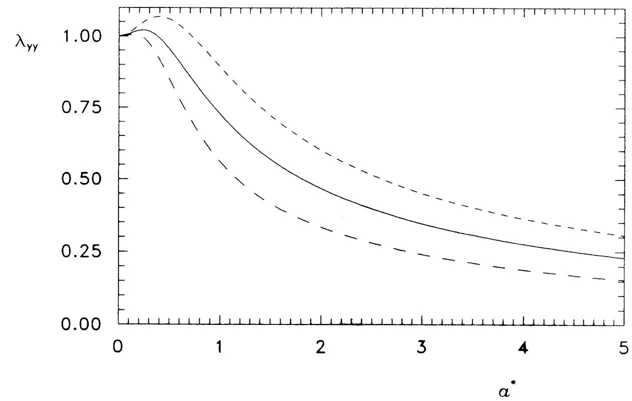

FIG. 1. Shear-rate dependence of the yy component of the thermal-conductivity tensor λ_{yy} for three interaction models: hard spheres interaction (—), Maxwell interaction (– – –), and VHP interaction (- - -).

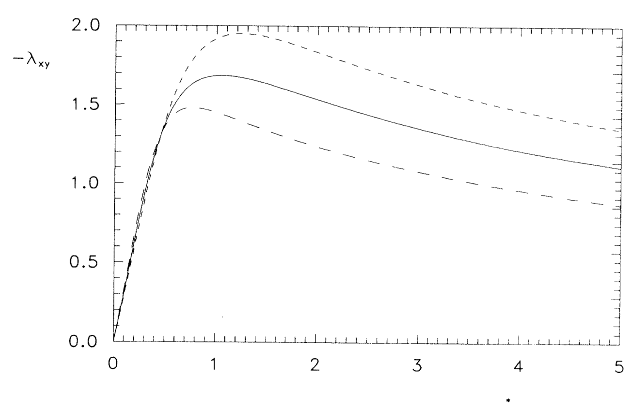

FIG. 2. The same as in Fig. 1, but for $-\lambda_{xy}$.

for the heat flux with those derived in the steady Couette flow [10] from the BGK equation. While in the latter case the solution to the BGK model is not restricted to small temperature gradients, our description only applies for weak thermal gradients. However, in both descriptions the heat flux always obeys a generalized Fourier's law with a shear-rate dependent thermal conductivity. On the other hand, the reduced thermal-conductivity tensor obtained here depends on the potential interaction while in the steady Couette flow is a universal function (independent of the potential model) of the shear rate. Although the energy transport presents different general properties in both steady shear-flow problems, it would be interesting to assess the numerical differences between them. This comparison is in the same spirit as the one carried out recently for the shear viscosity in both situations by using computer simulation methods [15] as well as by kinetic theory results [16]. Here, the comparison is restricted to the reduced component λ_{yy} since the temperature gradient taken in Ref. [10] is parallel to the y axis. By taking into account the same type of considerations as those reported in Ref. [16], we consider here the shear-rate dependence of the function $\varphi = (\lambda_{yy}^{\rm USF}/\lambda_{yy}^{\rm SCF})$. The superscripts USF and SCF refer to uniform shear flow and steady Couette flow, respectively. The shape of this function is plotted in Fig. 3. The coefficient $\lambda_{yy}^{\rm USF}$ corresponds here to the one computed in the VHP case, where our results are valid even for large temperature gradients. It is evident from Fig. 3 that both transport coefficients are very different beyond the Navier-Stokes limit. For instance, the super-Burnett contribution to the thermal conductivity takes the value $-\frac{18}{5}$ for the steady Couette flow whereas it takes the value $\frac{19}{5}$ in the uniform shear flow for the VHP interaction. For large shear rates, the thermal-conductivity coefficient exhibits different asymptotic behaviors. Thus, $\lambda_{yy}^{\rm USF} \sim a^{*-2/3}$, while $\lambda_{yy}^{\rm SCF} \sim a^{*-2} \ln a^*$. Figure 3 shows that the decreasing of the thermal conductivity as the shear rate increases is more noticeable in the steady Couette flow than in the uniform shear flow. It is clear that the origin of these discrepancies lies in the fact that both shear-flow states are macroscopically different. It must be noticed that these differences are more important than the ones obtained in the case of the shear viscosity [16].

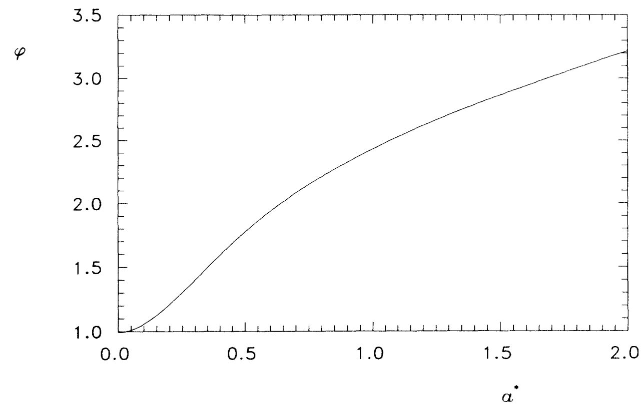

FIG. 3. Shear-rate dependence of the ratio of thermal conductivities $\varphi = (\lambda_{yy}^{\rm USF}/\lambda_{yy}^{\rm SCF})$.

It should be apparent that the derivation of explicit expressions for the transport properties involved in a nonequilibrium problem may prove to be useful for analyzing computer simulation results. While this approach in the case of self-diffusion and diffusion tensors under uniform shear flow has been exploited, we are not aware of the availability of similar simulation results for the thermal-conductivity tensor. We hope that the present work may serve to stimulate the performance of simulations of energy transport under shear flow. Finally, it must be emphasized that although our results were derived from the BGK model we expect that similar conclusions could be drawn out from the Boltzmann equation, at least for Maxwell molecules. Work along this line is in progress.

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