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Effect of energy nonequipartition on the transport properties in a granular mixture

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Abstract The Boltzmann kinetic theory is used to analyze the effect of energy nonequipartition on the pressure and the shear viscosity of a granular binary mixture under simple shear flow. Theory and Monte Carlo simulations show that both quantities exhibit a *non-monotonic* behaviour with the mass ratio in contrast to the predictions made from previous theories based on the equipartition assumption. Our results agree qualitatively well with recent molecular dynamics simulations performed by Alam and Luding [Granular Matter 4, 139 (2002)].

Keywords Kinetic and transport theory of gases, Monte Carlo simulation, Simple shear flow, Granular mixture

In a recent paper, Alam and Luding [1] have performed molecular dynamics simulations of a granular binary mixture under simple shear flow to assess the effect of energy nonequipartition on the transport coefficients (pressure and viscosity). Their main finding is that the pressure and viscosity exhibit a *non-monotonic* behaviour with the mass ratio whereas the theoretical predictions with the equipartition assumption suggest a *monotonic* dependence. They also propose a simplified model which takes as input parameters the expression of the shear viscosity η derived by Willits and Arnarson [2] for nearly elastic particles and the expression of the temperature ratio γ obtained by Barrat and Trizac [4] for a driven granular gas. In spite of these approximations, the model captures qualitatively well the main trends observed in the simulations. However, given that the expressions of η and γ chosen by Alam and Luding [1] do not coincide with those obtained in the simple shear flow problem, it would be interesting to reexamine the conclusions found by Alam and Luding [1] when the correct expressions for the temperature ratio and the shear viscosity are taken into account.

In this communication we revisit the issue studied by Alam and Luding [1] by using a recent *multitemperature* kinetic theory [5] for a granular binary mixture engaged in simple shear flow. Due to the complexity of the problem, the kinetic theory is restricted to the low-density regime in which case the velocity distribution functions f_i for the two species verify a set of two coupled nonlinear Boltzmann equations. This is the price to be paid for offering a quite refined theory. Although the Boltzmann equation is analytically solved by the moment method in the leading Sonine approximation, the corresponding theoretical predictions compare quite well with Monte Carlo simulations [5,6].

Let us consider a granular binary mixture composed by smooth inelastic disks or spheres of masses m_1 and m_2 and diameters σ_1 and σ_2. Collisions between particles are inelastic and characterized by three constant (independent) restitution coefficients α_{11}, α_{22}, and $\alpha_{12} = \alpha_{21}$, where $\alpha_{ij} \leq 1$ refers to the restitution coefficient for collisions between particles of species i and j. The mixture is under simple shear flow, namely, a macroscopic state with a constant linear velocity profile $\mathbf{U} = \mathsf{a} \cdot \mathbf{r}$, where $a_{k\ell} = a\delta_{kx}\delta_{\ell y}$, a being the constant shear rate. In addition, the partial densities n_i and the (global) granular temperature T are uniform. The time evolution of the temperature T arises from the balance of two competing effects: viscous heating and collisional cooling. When both mechanisms cancel each other, the system reaches a steady state and the temperature achieves a constant value. This steady state is what we want to analyze here.

From a microscopic point of view, the simple shear flow problem becomes spatially uniform in the local Lagrangian frame moving with the flow velocity $\mathbf{U}$. In this frame, $f_i(\mathbf{r}, \mathbf{v}) \to f_i(\mathbf{V})$, where $\mathbf{V} = \mathbf{v} - \mathbf{U}$ is the peculiar velocity. Under these conditions, the set of Boltzmann kinetic equations read

$$-aV_y \frac{\partial}{\partial V_x} f_i(\mathbf{V}) = \sum_j J_{ij}[\mathbf{V}|f_i, f_j] \ , \tag{1}$$

where the Boltzmann collision operator $J_{ij}\left[\mathbf{V}|f_i, f_j\right]$ is

$$J_{ij}\left[\mathbf{V}_1|f_i, f_j\right] = \sigma_{ij}^{d-1} \int d\mathbf{V}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \times \left[\alpha_{ij}^{-2} f_i(\mathbf{V}_1') f_j(\mathbf{V}_2') - f_i(\mathbf{V}_1) f_j(\mathbf{V}_2)\right] . \tag{2}$$

Here, d is the dimensionality of the system, $\sigma_{ij} = (\sigma_i + \sigma_j)/2$, $\widehat{\boldsymbol{\sigma}}$ is a unit vector along their line of centers, Θ

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is the Heaviside step function and $\mathbf{g}_{12} = \mathbf{V}_1 - \mathbf{V}_2$. In addition, the primes on the velocities denote the initial values $\{\mathbf{V}_1', \mathbf{V}_2'\}$ that lead to $\{\mathbf{V}_1, \mathbf{V}_2\}$ following a binary collision: $\mathbf{V}_1' = \mathbf{V}_1 - \mu_{ji}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$ and $\mathbf{V}_2' = \mathbf{V}_2 + \mu_{ij}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$. Here, $\mu_{ij} = m_i/(m_i+m_j)$.

The most relevant transport properties in a shear flow problem are obtained from the pressure tensor $\mathsf{P} = \mathsf{P}_1 + \mathsf{P}_2$, where P_i is the partial pressure tensor of the species i given by

$$\mathsf{P}_i = m_i \int d\mathbf{V}\mathbf{V}\mathbf{V} f_i(\mathbf{V}) \ . \tag{3}$$

The trace of P_i defines the partial temperatures T_i as $T_i = \mathrm{Tr}\mathsf{P}_i/dn_i$. These temperatures measure the mean kinetic energy of each species. The global temperature of the mixture (which is the relevant one at a hydrodynamic level) is $T = x_1T_1 + x_2T_2$, where $x_i = n_i/(n_1+n_2)$ is the mole fraction of species i. The elements of the pressure tensor P_i can be obtained by multiplying the Boltzmann equation (1) by $m_i\mathbf{V}\mathbf{V}$ and integrating over $\mathbf{V}$. The result is

$$a_{km}P_{i,m\ell} + a_{\ell m}P_{i,mk} = \sum_j A_{ij,k\ell} \ , \tag{4}$$

where we have introduced the collisional moments A_{ij} as

$$\mathsf{A}_{ij} = m_i \int d\mathbf{V}\mathbf{V}\mathbf{V} J_{ij}[\mathbf{V}|f_i, f_j] \ . \tag{5}$$

From Eq. (4), in particular, one gets the balance equation for the partial temperature T_i

$$aP_{i,xy} = -\frac{d}{2}p_i\zeta_i \ , \tag{6}$$

where $p_i = n_iT_i$ is the partial pressure of species i and $\zeta_i = \sum_j \zeta_{ij}$ is the cooling rate for the partial temperature T_i, with

$$\zeta_{ij} = -\frac{1}{dn_iT_i}\int d\mathbf{V} m_i V^2 J_{ij}[\mathbf{V}|f_i, f_j] \ . \tag{7}$$

According to Eq. (6), the (steady) partial temperature in the simple sear flow problem can be obtained by equating the viscous heating term $aP_{i,xy}$ with the collisional cooling term $(d/2)p_i\zeta_i$.

The determination of ζ_{ij} and A_{ij} requires the knowledge of the velocity distribution functions f_i. This is a quite formidable task even in the one-component case. However, as in the elastic case, one expects to get a good estimate of A_{ij} and ζ_{ij} by taking the leading term in an expansion of f_i in Sonine polynomials. Thus, we take the approximation $f_i(\mathbf{V}) \to f_{i,M}(\mathbf{V})\left[1 + \mathsf{C}_i : \mathsf{D}_i(\mathbf{V})/2T_i\right]$, where $\mathsf{C}_i = (\mathsf{P}_i/p_i) - \mathsf{1}$ and $\mathbf{D}_i(\mathbf{V}) = m_i\left[\mathbf{V}\mathbf{V} - (V^2/d)\mathsf{1}\right]$. Here, $\mathsf{1}$ is the $d\times d$ unit tensor and $f_{i,M}$ is a Maxwellian distribution at the temperature of the species i, i.e.,

$$f_{i,M}(\mathbf{V}) = n_i\left(\frac{m_i}{2\pi T_i}\right)^{d/2}\exp\left(-\frac{m_iV^2}{2T_i}\right) \ . \tag{8}$$

With this approximation, the collisional moments A_{ij} and the cooling rates ζ_{ij} can be explicitly evaluated. The details of these calculations have been published elsewhere [5,7] so only the results are quoted here. The results are

$$\begin{aligned}\mathsf{A}_{ij} = &-\frac{2\pi^{(d-1)/2}}{d\Gamma(d/2)}m_in_in_j\mu_{ji}\sigma_{ij}^{d-1}\left(\frac{2T_i}{m_i}+\frac{2T_j}{m_j}\right)^{3/2}\\ &\times(1+\alpha_{ij})\left\{\mu_{ji}\left[\frac{T_i-T_j}{(m_j/m_i)T_i+T_j}+\frac{1-\alpha_{ij}}{2}\right]\mathsf{1}\right.\\ &+\frac{1}{1+(m_iT_j/m_jT_i)}\left[\frac{\mathsf{C}_i-\mathsf{C}_j}{1+(m_jT_i/m_iT_j)}\right.\\ &\left.\left.+\frac{d+3}{2(d+2)}\lambda_{ij}\left(\mathsf{C}_i+\frac{m_iT_j}{m_jT_i}\mathsf{C}_j\right)\right]\right\} \ ,\end{aligned} \tag{9}$$

$$\begin{aligned}\zeta_{ij} = &\frac{2\pi^{(d-1)/2}}{d\Gamma(d/2)}\frac{m_in_j}{T_i}\mu_{ji}^2\sigma_{ij}^{d-1}\left(\frac{2T_i}{m_i}+\frac{2T_j}{m_j}\right)^{3/2}(1+\alpha_{ij})\\ &\times\left[\frac{T_i-T_j}{(m_j/m_i)T_i+T_j}+\frac{1-\alpha_{ij}}{2}\right] \ ,\end{aligned} \tag{10}$$

where

$$\lambda_{ij} = 2\mu_{ji}\frac{T_i-T_j}{(m_j/m_i)T_i+T_j} + \frac{\mu_{ji}}{d+3}(2d+3-3\alpha_{ij}) \ . \tag{11}$$

Substitution of (9) into the set of equations (4) allows one to get the partial pressure tensor P_i in terms of the temperature ratio $\gamma = T_1/T_2$ and the parameters of the mixture. The temperature ratio can be obtained from Eq. (6) as

$$\gamma = \frac{x_2\zeta_2P_{1,xy}}{x_1\zeta_1P_{2,xy}} \ . \tag{12}$$

When the expressions of P_i and ζ_i are used in Eq. (12), one gets a *closed* equation for the temperature ratio γ, that can be solved numerically. In Fig. 1 we plot γ versus the diameter ratio σ_1/σ_2 for a two-dimensional granular gas with $x_1 = 1/2$ and two different values of α. The symbols refer to the simulation data obtained from the Direct Simulation Monte Carlo (DSMC) method [6]. Here, we have assumed $\alpha_{ij} = \alpha$ and equal mass densities $[m_1/m_2 = (\sigma_1/\sigma_2)^2]$. The predictions due to Barrat and Trizac [4] for the homogeneous steady state driven by a white noise thermostat have been also included. As said before, this expression was used by Alam and Luding [1] to obtain the pressure and the shear viscosity coefficients in the simple shear flow problem. It is clearly seen that while our theoretical results agree quite well with simulation data, Barrat and Trizac's theory overestimates them especially for large mass ratio. This disagreement is not surprising since the situation analized by Barrat and Trizac (homogeneous driven state) is different from the one studied here.

Let us now consider the transport coefficients. As in Ref. [1], for a low-density gas we introduce the reduced pressure p^* and the reduced shear viscosity η^* as

$$p^* = \frac{p\nu^2}{\rho_1v_0^2a^2} \ , \tag{13}$$

$$\eta^* = \frac{\eta\nu^2}{\rho_1v_0^2a} \ , \tag{14}$$

where $p = nT$, $\rho_1 = m_1n_1$, $\eta = -P_{xy}/a$, $P_{xy} = P_{1,xy} + P_{2,xy}$ and $\nu = [\pi^{(d-1)/2}/\Gamma(d/2)]n\sigma_{12}^{d-1}v_0$ is an effective

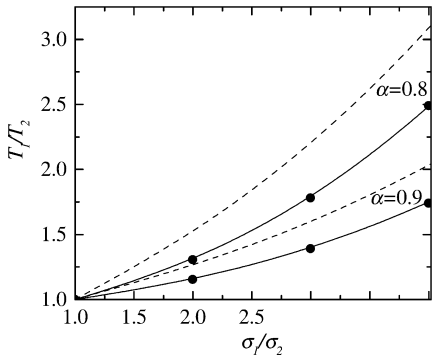

Fig. 1. Plot of the temperature ratio T_1/T_2 as a function of the size ratio $\sigma_1/\sigma_2 = (m_1/m_2)^{1/2}$ for a two-dimensional system in the case $x_1 = 1/2$ and two different values of the restitution coefficient α: $\alpha = 0.9$ and $\alpha = 0.8$. The solid lines are our theoretical predictions while the symbols refer to the DSMC results. The dashed lines correspond to the results obtained from the theory of Barrat and Trizac [4] for a granular mixture driven by a white noise thermostat

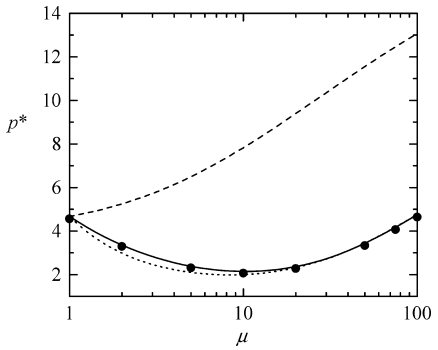

Fig. 2. Plot of the reduced pressure $p^* = p\nu^2/\rho_1 v_0^2 a^2$ versus the mass ratio $\mu = m_1/m_2$ for a two-dimensional system with $\sigma_1 = \sigma_2$, $x_1 = 1/2$ and $\alpha = 0.9$. The solid line corresponds to our theoretical predictions, the dotted line refers to our theory but using the expression of Barrat and Trizac [4] for the temperature ratio $\gamma = T_1/T_2$, and the dashed line is the result obtained from our model by assuming the equality of the partial temperatures $\gamma = 1$. The symbols are the DSMC results

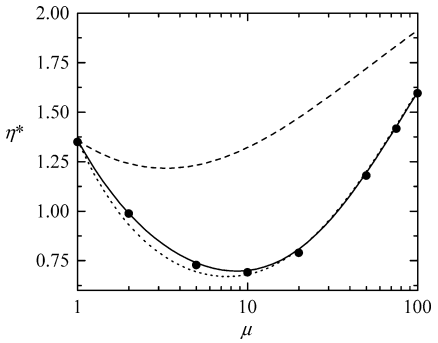

Fig. 3. Plot of the reduced shear viscosity $\eta^* = \eta\nu^2/\rho_1 v_0^2 a$ versus the mass ratio $\mu = m_1/m_2$ for a two-dimensional system with $\sigma_1 = \sigma_2$, $x_1 = 1/2$ and $\alpha = 0.9$. The solid line corresponds to our theoretical predictions, the dotted line refers to our theory but using the expression of Barrat and Trizac [4] for the temperature ratio $\gamma = T_1/T_2$, and the dashed line is the result obtained from our model by assuming the equality of the partial temperatures $\gamma = 1$. The symbols are the DSMC results

collision frequency. In Figs. 2 and 3, we plot p^* and η^*, respectively, as a function of the mass ratio $\mu = m_1/m_2$ for an *equal-size* ($\sigma_1 = \sigma_2$) binary mixture of disks ($d = 2$) with $x_1 = 1/2$ and $\alpha = 0.9$. This was the case considered in Ref. [1]. We have also included the predictions for p^* and η^* given by our theory but taking the expression of γ provided by Barrat and Trizac [4]. We observe again in both figures an excellent agreement between our theory and the DSMC results even for very disparate values of the mass ratio. With respect to the influence of energy nonequipartition, Fig. 2 shows that p^* presents a *non-monotonic* behaviour with the mass ratio whereas the theoretical predictions with the equipartition assumption *monotonically* increase with μ. In the case of the shear viscosity, the above trends are not completely followed as seen in Fig. 3, since both theories (with and without energy nonequipartition) suggest a *non-monotonic* dependence of η^* on μ. However, at a quantitative level, the influence of energy nonequipartition is quite significant over the whole range of mass ratios considered. Although the solid fraction $\Phi = 0.1$ considered in the simulations of Ref. [1] prevent us to make a quantitative comparison (since our results apply strictly only for $\Phi = 0$), we observe that the *non-monotonic* dependence of p^* and η^* on μ found in the molecular dynamics simulations agrees qualitatively well with the one obtained here from the Boltzmann kinetic theory. Thus, for instance, the minimum values of p^* and η^* are close to $\mu = 10$ in both dilute and dense cases. On the other hand, the predictions for the transport properties given from our theory by taking the Barrat and Trizac expression of γ are quite close to those obtained from the actual value of γ, especially for large mass ratios.

It must be noted that the expression of the viscosity chosen by Alam and Luding [1] differs from the one used here for the simple shear flow, even if one assumes in our theory the equipartition of energy (i.e., $\gamma = 1$). While the former has been derived from the Chapman-Enskog expansion around the local equilibrium distribution, our description holds for a situation where the (reduced) shear rate a/ν is coupled to the restitution coefficients α_{ij}. This is the reason for which the conventional theories (which are based on energy equipartition) [2] give a monotonic behavior of η^* with μ in contrast to the result obtained here (cf. Fig. 3) when one takes $\gamma = 1$ [8].

In conclusion, the Boltzmann kinetic theory applied to a granular binary mixture under simple shear flow predicts a *non-monotonic* behaviour of the pressure and the viscosity on the mass ratio. This conclusion agrees qualitatively well with recent molecular dynamics simulations performed by Alam and Luding [1]. In addition, although the Boltzmann solution has been obtained by considering only the leading Sonine approximation to the distribution function, its accuracy has been widely confirmed by Monte Carlo simulations. Given that the main limitation of the results presented here is their restriction to the low-density regime, we plan to extend the above calculations to higher densities by using the revised Enskog theory. This would allow us to make a more quantitative comparison with the simulation data found by Alam and Luding [1]. Work along this line is in progress.

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8. Note that conventional theories deal with moderately dense fluids so that the solid fraction can play an important role in the dependence of the (reduced) pressure and (reduced) viscosity on the mass ratio. In this sense, it is possible that a consistent extension of our theory to dense gases also predicts a monotonic decay of p^* and η^* with μ when one takes energy equipartition