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F. Vega Reyes and V. Garzó

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Energy Non-Equipartition in a System with a Granular Impurity Under Couette-Fourier Flow

F. Vega Reyes and V. Garzó

Departamento de Física, Universidad de Extremadura, 06071 Badajoz, Spain

Abstract. We show in this work the energy non-equipartition (difference in temperature) of a *sheared* granular mixture composed by two sets of smooth spheres each one having a characteristic particle mass and diameter. We assume that the concentration of one of the species (species 1, or “impurity”) is negligible (tracer limit). In these conditions, the state of the excess component 2 is not disturbed by the presence of of the tracer species while the collisions among tracer particles themselves can be neglected. The system (granular gas plus impurities) is driven in a Couette-Fourier geometry: a granular mixture enclosed between two infinite parallel walls from which we heat and eventually shear the system. More specifically, we focus on a special class of steady states with uniform heat flux, in which case an exact balance between viscous heating and collisional cooling throughout the system exists. The temperature ratio T_1/T_2 is obtained by following two complementary routes: an analytical solution to the Boltzmann and Boltzmann-Lorentz kinetic equations from Grad’s moment method and a numerical solution of the above equations by means of the direct simulation Monte Carlo (DSMC) method. Comparison between theory and simulation shows in general good agreement, even for strong values of dissipation.

Keywords: Granular gases, energy non-equipartition, impurity segregation, Couette flow

PACS: 45.70.Mg, 05.20.Dd, 47.50.-d, 51.10.+y

INTRODUCTION

In physics, the term *granular* is regularly used for systems composed of mesoscopic particles that collide inelastically with each other; i. e., energy is not conserved in the collisions. These particles are what we know as *grains* and hence the term *granular*. More specifically, we focus in this work in a *kinetic* granular system, where the dynamics of the grains is determined by short collision times, since all grains have a large enough kinetic energy at all times. The countertype would be a *frictional* granular system, for which grains do not all have enough kinetic energy at all times and clusters of them tend to remain in contact longer times [1, 2]. Kinetic granular systems usually have a large number of particles and in many cases coarse-grained properties can completely describe the system, in the same way as in classic soft condensed matter [3] and in fluid mechanics [4]. For this reason, kinetic granular matter has been extensively studied in the fields of both statistical and fluid mechanics [5, 6, 7, 8]. Most theoretical studies in the context of both branches of physics have taken advantage of the existing background for systems with atomic entities, for which particle collisions are elastic (energy is conserved in collisions) and equilibrium thermodynamics may apply [9, 8, 10]. Examples of this connection may be found in a variety of problems, such as disordered-ordered phase transitions [11, 12], laminar flows [13], diffusion [14], hydrodynamic instabilities [15], suspensions [16], pattern formation [17, 18], segregation [19], geologic surface transport [20], etc.

A kinetic granular system is usually called *granular gas* if it has a low enough density, so that a Boltzmann-type or Enskog-type kinetic equation for the system applies [6]. The homogeneous cooling state (HCS) in granular gases is the counterpart of the thermodynamic equilibrium state (characterized by a Maxwellian distribution function) of systems with elastic particle collisions. The HCS is characterized by homogeneous density and temperature, but the temperature decreases in time due to collisional cooling. Thus, the HCS plays in granular gases the role of the zeroth order term, in the same way the equilibrium state does for perturbative solutions of non-uniform gases [21, 22].

However, and contrary to the thermodynamic equilibrium state, the HCS is inherently unsteady and besides highly unstable [23]. Indeed, let us imagine an isolated kinetic granular system, initially homogeneous, and characterized by a random distribution of velocities. Due to loss of kinetic energy at particle collisions, the global initial temperature (average kinetic energy) of the system decreases monotonically in time. It is now known that this decrease is very precisely described by Haff’s law [24]. Hence, the homogeneous state for kinetic granular systems is inherently unsteady. At first, homogeneous density and temperature may be kept. However, fluctuations in the collision frequency may result in the formation of a cluster, since if more collisions per unit time occur in one region, the particles will

have less kinetic energy there, and thus they will tend to stay there longer times together. In this way, this collision frequency/density fluctuation feeds itself and the homogeneous state becomes unstable forming clusters. This is the so-called clustering instability [23]. Thus, the fact that this base homogeneous state is inherently unsteady and unstable finally results in significant differences of the behavior of granular systems with respect to molecular gases in transport problems. Moreover, since the elastic limit can be recovered in granular dynamics theories, results from equilibrium statistical mechanics [25] and classic fluid mechanics [13] can be viewed as special cases of a more general problem which takes into account the possibility of inelastic collisions.

On the other hand, most situations of practical interest for kinetic granular gases involve some kind of energy input, generally from the boundaries of the system. In this way, spatial gradients are generated in the bulk of the system, which allows for the system to achieve a steady inhomogeneous state. When it comes to studying steady states, the traditional geometries studied in fluids are also used for kinetic granular systems [5]. For instance, the flow in a system enclosed by and excited from two infinite parallel walls. These walls may act as only temperature sources (Fourier flow problem) or as shear and temperature sources (Couette flow problem). In recent works [13, 26, 27], the different types of flows that can appear for granular systems in these geometries have been classified. Moreover, the simple (or uniform) shear flow (USF), that is the paradigmatic steady flow in kinetic granular systems [28] has been generalized to be described as a special case of a more general class of flows called “LTu” class (because temperature (T) profiles are linear vs. flow velocity (u) profiles) [13, 27].

The USF in granular gases is a steady laminar planar flow (more concretely, a Couette flow type) characterized by constant density and temperature profiles and a linear flow velocity profile. It may become unstable but it has wide regions of stability [15]. Contrary to what happens in a traditional gas, the USF in a granular gas is stationary. Because of its simplicity (it has a linear flow velocity and constant temperature and density), this type of flow has been extensively studied and is used as a reference state for studying more complex problems in granular flows [29, 30]. Furthermore, recent results have shown that there is a connection between the USF and the classic Fourier flow in an elastic gas, through the LTu class of granular flows. However, due to inelastic cooling, the LTu and the USF (which is a special case of LTu flow) are inherently non-Newtonian, and a Navier-Stokes approach is in general not useful [13]. Furthermore, in our recent works [13, 27], we proved also that the same USF may be generated with different boundary conditions: the USF in bounded systems is not distinguishable from the USF in unbounded systems (where usually Lees-Edwards boundary conditions are used [28]). This means that the same generalized transport coefficients and hydrodynamic steady profiles are measured in bounded and unbounded systems. This supports the procedure of solving the hydrodynamic steady base states and describing the boundary conditions as separate theoretical problems [5, 26], just in the same way it is usually done in fluid dynamics [31]. Again, we find here another parallelism between granular and classic fluid dynamics.

ENERGY NON-EQUIPARTITION IN KINETIC GRANULAR SYSTEMS

One of these generalizing parallelism may be identified in the question of the granular temperature of the homogeneous state for mixture systems; i.e., systems composed by different sets of identical particles (we can call these sets *species*). With regards to this, and for equilibrium systems, the characteristic temperatures of all species are equal in the homogeneous state no matter how different their properties are. However, this is not the case for granular mixtures. One important theoretical result, verified in computer simulations [32, 33] and experiments [34], is that all temperature ratios (temperature of one of the species over the total granular temperature) for the HCS are constant (independent of time) but different from one. In general, the temperature ratios exhibit a complex dependence on the coefficients of restitution and the parameters of the mixture (masses, sizes and concentration) [35]. Thus, we say there is *energy non-equipartition* in granular mixtures in the HCS. Additionally, an important consequence of constant temperature ratio is that in HCS all species cool at the same rates [35]. Thus, we talk in general of *energy non-equipartition* when different parts or dimensions of the system are characterized by different temperatures. Another important example is a vibrated granular gas with a granular impurity, where energy non-equipartition also has been observed [36].

As a matter of fact, energy non-equipartition is ubiquitous in kinetic granular systems. It is present even in certain monocomponent systems. In quasi-2D kinetic granular systems, we may observe a whole series of phase transitions characterized by different symmetry breaks [12, 25, 37, 38]. For instance, there exists a transition from a single disordered fluid-like phase to a two-phase coexistence, with a second ordered phase that is colder than the disordered phase. Thus, we may observe steady states where the temperature has at least two regions/phases characterized by homogeneous, but different, temperatures each. Interestingly, other phase transitions observed in kinetic granular systems follow a Kosterlitz-Thouless melting scenario, which implies that energy non-equipartition appears only as

localized thermal defects [37].

But the question arising is: how is energy non-equipartition for granular binary mixtures in *steady states*? We will analyze here the properties of the temperature ratio in the aforementioned generalized-USF; the LTu flow class. More specifically, we consider the tracer limit case, namely, a binary mixture where the concentration of one of the species (say for instance, species 1) is negligible.

Let us consider a system of two sets of inelastic smooth hard spheres characterized by masses m_1 and m_2 and diameters σ_1 and σ_2 . In the tracer limit, the collisions among tracer (or impurity) particles themselves can be neglected while the state of the excess species 2 is not perturbed by the presence of the impurities. Consequently, we may neglect $1-1$ collisions in the kinetic equation for the one-particle distribution function f_1 of the tracer particles while only $2-2$ collisions will be considered in the kinetic equation for the one-particle distribution function f_2 of the gas particles [39]. In addition, in the tracer limit, the total granular of the system T coincides with the temperature of the gas particles T_2 , i.e., $T \simeq T_2$. A previous work [40] on the LTu flow in the tracer limit showed that the temperature ratio $\chi \equiv T_1/T_2$ is again in general different from 1 for steady Couette flows. We also showed that the value of χ is homogeneous even for highly inhomogeneous steady states. Furthermore, our theoretical results imply that the LTu class exists as a steady base state also for the granular impurity [40] and that its hydrodynamic properties are independent of the imposed thermal gradient $\Delta T/\Delta L$ (wall temperature difference ΔT over the system size ΔL). In this work, we will confirm by means of the DSMC method [41] that χ is in effect constant for LTu flows. We will also show from computer simulations that χ is independent of the imposed thermal gradient, just like the other generalized hydrodynamic properties for a monocomponent granular gas in the LTu state [13, 26].

In addition, our simulations also indicate that the impurity always mimics the characteristic LTu flow velocity profile of the granular bath. This, together with $\chi \equiv \text{const}$ and independent from $\Delta T/\Delta L$, already implies that the LTu state occurs as a base state for the same set of boundary conditions for the flow velocity and the temperature that for the granular gas [40]. Another interesting result obtained in this paper is that the temperature ratio remains constant even if the impurity shows *segregation* [42]; i.e., if the concentration of the impurity is not homogeneous and so, the state of the impurity is not in its LTu base state. The departure from the base state may be signaled by an inhomogeneous partial hydrostatic pressure (p_1), since constant hydrostatic pressure p_2 is a generic property of planar Couette flows [13, 43].

GRANULAR IMPURITY UNDER LTU FLOWS

As mentioned before, we are interested in the dynamics of an impurity immersed in a granular gas in the steady LTu flow. From a macroscopic point of view, this state is characterized by the hydrodynamic profiles

$$p_2 = n_2 T_2 \equiv \text{const}, \quad (1)$$

$$v_2^{-1} \partial_y u_{2,x} = a \equiv \text{const}, \quad (2)$$

$$v_2^{-1} \partial_y T_2 \equiv \text{const}. \quad (3)$$

Here, a is the constant shear rate (which is a function of the coefficient of restitution α_{22} in the steady state) and $v_2 \propto n_2 \sqrt{T_2}$ is an effective collision frequency for gas particles.

In the tracer limit, the kinetic equations describing the system are the (closed) Boltzmann equation for the velocity distribution function f_2 of the granular gas and the Lorentz-Boltzmann equation for the velocity distribution function f_1 of the impurity. These equations are given, respectively, by

$$-a V_y \frac{\partial f_2}{\partial V_x} = J_{22}[f_2, f_2], \quad (4)$$

$$-a V_y \frac{\partial f_1}{\partial V_x} = J_{12}[f_1, f_2], \quad (5)$$

where

$$J_{ij}[\mathbf{v}_1 | f_i, f_j] = \sigma_{ij}^{d-1} \int d\mathbf{v}_2 \int d\hat{\sigma} \Theta(\mathbf{g} \cdot \hat{\sigma}) (\mathbf{g} \cdot \hat{\sigma}) \left[\alpha_{ij}^{-2} f_i(\mathbf{v}'_1) f_j(\mathbf{v}'_2) - f_i(\mathbf{v}_1) f_j(\mathbf{v}_2) \right]. \quad (6)$$

Here, $\sigma_{ij} = (\sigma_i + \sigma_j)/2$, $\hat{\sigma}$ is a unit vector along the line of centers, Θ is the Heaviside step function, and $\mathbf{g} = \mathbf{v}_1 - \mathbf{v}_2$ is the relative velocity. 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 the

binary collision:

$$\begin{aligned} \mathbf{v}'_1 &= \mathbf{v}_1 - \mu_{ji} \left(1 + \alpha_{ij}^{-1}\right) (\mathbf{g} \cdot \hat{\boldsymbol{\sigma}}) \hat{\boldsymbol{\sigma}}, \\ \mathbf{v}'_2 &= \mathbf{v}_2 + \mu_{ij} \left(1 + \alpha_{ij}^{-1}\right) (\mathbf{g} \cdot \hat{\boldsymbol{\sigma}}) \hat{\boldsymbol{\sigma}}, \end{aligned} \quad (7)$$

where $\mu_{ij} \equiv m_i / (m_i + m_j)$. Moreover, $\mathbf{V} = \mathbf{v} - \mathbf{u}_2$ is the peculiar velocity and $u_{2,\ell} = ay\delta_{\ell x}$ is the mean flow velocity of the gas particles. Note that the Boltzmann and Lorentz-Boltzmann equations (4) and (5), respectively, become homogeneous in the LTu flow when we refer the velocities of the particles to a frame moving with the flow velocity \mathbf{u}_2 [39, 40].

The relevant rheological properties of the system are provided by the pressure tensor $P_{2,k\ell}$ of the excess gas and the partial pressure tensor $P_{1,k\ell}$ of the impurity. In terms of the distributions f_2 and f_1 , they are defined as

$$P_{2,k\ell} = \int d\mathbf{v} m_2 V_k V_\ell f_2(\mathbf{V}), \quad (8)$$

$$P_{1,k\ell} = \int d\mathbf{v} m_1 V_k V_\ell f_1(\mathbf{V}), \quad (9)$$

The hydrostatic pressure of the granular gas is defined as $p_2 = \frac{1}{d} P_{2,kk}$ while the partial pressure of the impurity is $p_1 = n_1 T_1 = \frac{1}{d} P_{1,kk}$. In the steady state, the temperature ratio χ can be easily obtained by multiplying both sides of Eq. (4) by $\frac{m_2}{2} V^2$ and of Eq. (5) by $\frac{m_1}{2} V^2$ and integrating over velocity. The result is

$$\chi = \frac{\zeta_2 P_{1,xy}}{\zeta_1 P_{2,xy}}, \quad (10)$$

where we have introduced the cooling rates ζ_2 and ζ_1 as

$$\zeta_2 = -\frac{m_2}{dn_2 T_2} \int d\mathbf{v} V^2 J_{22}[f_2, f_2], \quad (11)$$

$$\zeta_1 = -\frac{m_1}{dn_1 T_1} \int d\mathbf{v} V^2 J_{12}[f_1, f_2]. \quad (12)$$

Since ζ_i and $P_{i,xy}$ are proportional both to the partial density n_i , then the temperature ratio χ is not influenced by the specific form of the density profiles. Consequently, the temperature ratio should not vary when the density profile is perturbed due to segregation. We will prove through computer simulations that the values of χ are not sensitive to wall temperature difference nor segregation. This means that the same value of χ (as obtained from (10)) is observed for LTu flows at different boundary or segregation conditions, as long as the values of the parameters of the system (the coefficients of restitution α_{ij} , the mass ratio $\mu \equiv m_1/m_2$ and the size ratio $\omega \equiv \sigma_1/\sigma_2$) remain the same. This actually confirms that segregation indeed occurs for impurities under LTu flow, at constant heat flux, since Eq. (10) only applies for constant heat flux.

In order to get an explicit form for χ , the Grad's moment method [22] is employed to obtain the pressure tensors $P_{2,k\ell}$ and $P_{1,k\ell}$ and the cooling rates ζ_2 and ζ_1 [32, 44]. The explicit forms of these quantities in terms of the masses and sizes and the coefficients of restitution α_{22} and α_{12} are given in the Appendix A of Ref. [45]. Once the forms of the pressure tensors and the cooling rates are known, the temperature ratio χ is determined from the relation(10). As long as nonlinear terms in the irreversible fluxes [46] are not retained, the solution for χ does not depend on the magnitude of heat flux components.

COMPARISON BETWEEN GRAD'S SOLUTION AND DSMC RESULTS

In this Section, we compare the theoretical results for χ obtained from Grad's moment method with those obtained from the DSMC method. Technical details on the DSMC algorithm applied to the LTu flow may be found in Ref. [40]. Figure 1 shows the temperature ratio χ versus the (common) coefficient of restitution $\alpha \equiv \alpha_{22} = \alpha_{12}$ for $\omega = 1$ and four different values of the mass ratio μ ($\mu = 1/4, 1/2, 2$, and 4). The solid lines denote the theoretical results while symbols refer to simulation results. Several values of the temperature difference ΔT have been considered ($\Delta T = 0, 5$, and 10). Since Grad's solution is independent of $\Delta T/\Delta L$, we get just one line for different $\Delta T/\Delta L$ but same values of

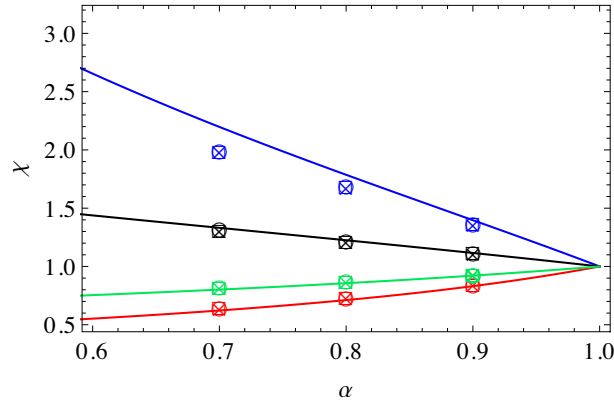


FIGURE 1. Temperature ratio $\chi \equiv T_1/T_2$ as a function of the (common) coefficient of restitution $\alpha \equiv \alpha_{22} = \alpha_{12}$ for $\omega = 1$, and four different values of the mass ratio $\mu \equiv m_1/m_2$: $\mu = 1/4$ (red), $\mu = 1/2$ (green), $\mu = 2$ (black), and $\mu = 4$ (blue). Lines correspond to Grad's theoretical results and symbols stand for DSMC results, for different wall temperature difference ΔT : circles stand for $\Delta T = 0$, crosses for $\Delta T = 5$ and squares for $\Delta T = 10$. For all simulations, $\Delta L = 15$.

the remaining parameters. Respect to simulation results, we can also notice that the values of χ are also independent of $\Delta T/\Delta L$, since no difference can hardly be detected for same color symbols. It is worth to point out also that the agreement between theory and simulation is excellent, except perhaps for $\mu = 4$ where the agreement is still quite good. This shows the reliability of Grad's solution to characterize the non-Newtonian behavior of the temperature ratio beyond the quasielastic limit (which means beyond the Navier-Stokes description in the steady LTu flow due to the coupling between dissipation and the reduced shear rate a).

To illustrate the differences between the theoretical results obtained here with those derived in the HCS [35], Fig. 2 compares both LTu and HCS theories (color and black lines respectively) with DSMC data (symbols). As we see, the Grad's solution approach is significantly better, specially in Fig. 2 (a) for heavier impurities, for which both theoretical solutions tend to separate and only Grad's prediction stays very close to the numerical solution.

Finally, we can now show that energy non-equipartition is not sensitive to impurity segregation. In figure 3 (a) we demonstrate that in effect there is segregation in the system, with $\Delta T = 10$, $\Delta L = 15$, $\omega = 1$ and $\alpha = 0.9$; the solid and open symbols corresponding to the χ values denoted in Fig. 1 by black ($\mu = 2$) and green ($\mu = 0.5$) squares, respectively. As we can see in Fig. 1, there is no difference at all between these values and the ones of the temperature ratio in the USF state (black and green circles at $\alpha = 0.9$). As we recall, by definition, there is no segregation in the USF since it is characterized by flat density profiles [39]. Similar observations were made for other LTu flows. Thus, it is very clear that the DSMC results prove that the temperature ratio χ is the same for the base states and for the corresponding segregation states. In Fig. 3 (b), we plot $\log(x_1)$ vs. $\log(T_2)$ where $x_1 = n_1/n_2$ stands for the relative density of the impurity. We observe that $\log(x_1)$ is a linear function of $\log(T_2)$, which is consistent with some recent theoretical results [47] obtained in the absence of shear flow.

CONCLUSIONS

We have studied the properties of the energy non-equipartition through the temperature ratio $\chi \equiv T_1/T_2$ for LTu flows for a range of values of the relevant parameters in the problem: the coefficients of restitution associated to the inelastic collisions (α_{12} for impurity-gas collisions and α_{22} for gas-gas collisions), and the mass ($\mu \equiv m_1/m_2$) and diameter ($\omega \equiv \sigma_1/\sigma_2$) ratios. The agreement found for the temperature ratio between Grad's theory [14, 45, 48] and DSMC is in general very good. Furthermore, we have found that for LTu flows the temperature ratio χ takes the same value for the same system parameter values whether there is segregation or not, which implies that the theoretical values of χ from the USF state (base state) may be used. This also implies that segregation from LTu flows occurs with no variation of heat flux since the theoretical condition for χ from Grad's theory uses the fact that heat flux is uniform for the LTu class.

Additionally, we have observed also that for LTu class, the flow velocity profile for the impurity is also identical to that of the granular gas even when segregation occurs. In summary, impurity segregation for LTu granular flows

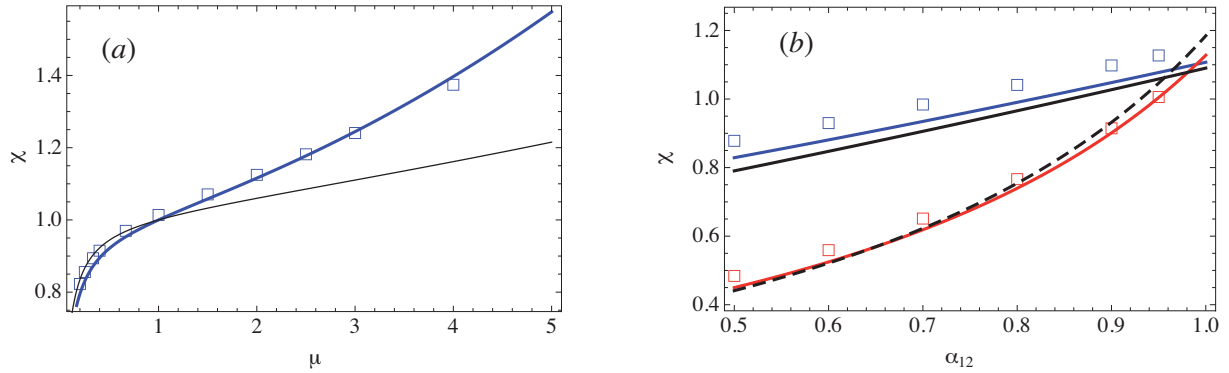


FIGURE 2. Temperature ratio χ for several configurations. Symbols stand for DSMC data, while color lines stand for Grad's theoretical results and black lines stand for the results obtained in the HCS. $\Delta T = 10, \Delta L = 15$. In the panel (a), χ is plotted versus the mass ratio μ , with $\alpha_{22} = \alpha_{12} = 0.9$ and $\omega = 1$; symbols stand for simulations while blue and black lines refer to the theoretical predictions obtained here and in the HCS. In the panel (b), χ is plotted as a function of α_{12} , with $\alpha_{22} = 0.9$ and $\omega = 2, \mu = 4$ (blue symbols: DSMC, blue lines: Grad's theory for LTu class, solid black line: HCS values) and $\omega = 1/2, \mu = 1/4$ (red symbols: DSMC, red line: Grad's theory for LTu class, and black-dashed line: HCS values)

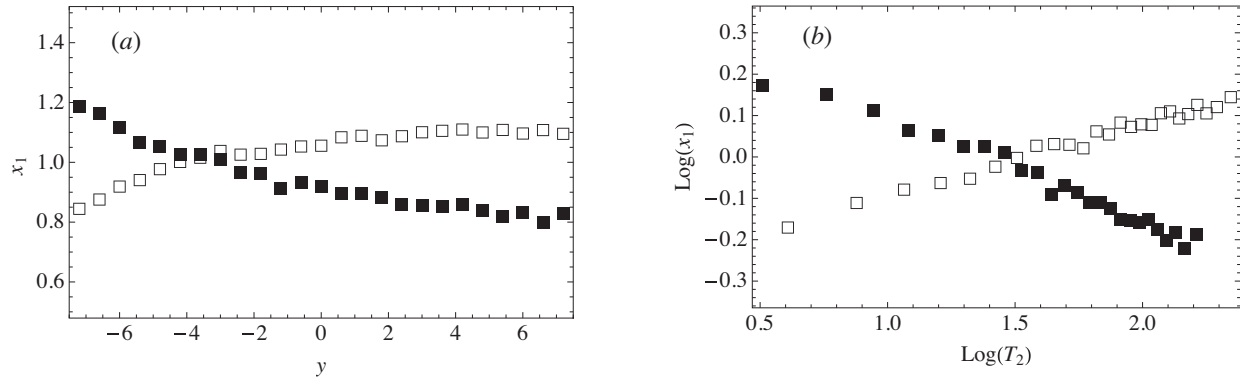


FIGURE 3. DSMC data for systems with impurity segregation. In the panel (a), we show the relative density $x_1 = n_1/n_2$ profile for an LTu state ($\Delta T = 10, \Delta L = 15$), with $\alpha_{22} = \alpha_{12} = 0.9, \omega = 1$, and $\mu = 2$ (solid symbols) and $\mu = 1/2$ (open symbols). In the panel (b), $\log(x_1)$ is plotted versus $\log(T_2)$ for the same systems as in the panel (a).

only changes the relative density profile properties, but keeps intact the peculiar properties of LTu flows: linear $T(u_{2,x})$ profile and uniform heat flux.

In general, the agreement found between theoretical (Grad's solution) and simulation (DSMC) values for χ is qualitatively good, being excellent for Grad's theory for all observed ranges of parameter values. The theoretical values for χ derived in the HCS [35] for equating the cooling rates do not show such a fine agreement. Thus, Grad's theory significantly improves the results for χ in the LTu flows.

We expect to apply the results derived here to analyze segregation by thermal diffusion in a sheared granular mixture. The idea is to take the forms of the Navier-Stokes transport coefficients [49] but replacing the temperature ratio χ of the HCS by the one obtained here from Grad's moment method. We also plan to check if the temperature ratio has also the same values independently of segregation for other Couette granular flows, such as LTy (for which heat flux is not uniform [26]).

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