Lack of energy equipartition in homogeneous heated binary granular mixtures

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We consider the problem of determining the granular temperatures of the components of a homogeneous binary heated mixture of inelastic hard spheres, in the framework of Enskog kinetic theory. Equations are derived for the temperatures of each species and their ratio, which is different from unity, as may be expected since the system is out of equilibrium. We focus on the particular heating mechanism where the inelastic energy loss is compensated by an injection through a random external force (“stochastic thermostat”). The influence of various parameters and their possible experimental relevance is discussed.

I. INTRODUCTION

Experimental and theoretical studies of rapid granular flows have hitherto mostly focused on assemblies of identical particles, either freely cooling when the energy loss due to inter-particle collisions is not compensated for, or driven in a non-equilibrium stationary state by various energy injection mechanisms. Recently however, interest has grown for the more complicated case of polydisperse systems. Theoretical investigations into the homogeneous cooling stage of a binary mixture have shown that the two components have different granular temperatures, even if their cooling rates are equal. Such a result, confirmed by detailed Monte Carlo simulations, is also obtained when the system is sheared, heated by the contact with an elastic granular gas maintained at fixed temperature $T$, or within the Maxwell model framework. Similarly, a tracer particle undergoing inelastic collisions with an equilibrium fluid at temperature $T$ reaches a granular temperature lower than $T$.

This violation of equipartition in a mixture, although in sharp contrast with the behaviour of molecular gases at equilibrium, is not unexpected: the terminology “granular temperature” for the kinetic energy of a granular gas has been coined from the equivalence of temperature and kinetic energy in an elastic gas, but does not have any thermodynamical status in out-of-equilibrium systems like inelastic granular gases.

In recent experiments, the granular temperatures have been measured for binary mixtures, both in 3D vibro-fluidized granular beds and in 2D strongly vibrated granular gases. Both studies reported a clear violation of equipartition with a temperature ratio quite insensitive to the relative densities of the two species.

The present article aims at providing a simple theoretical framework where the temperature ratio is readily obtained in a non-equilibrium steady state (NESS). This allows to investigate the influence of many parameters which can be difficult to tune experimentally, such as the masses, sizes, densities and inelasticities of the beads. We consider analytically a heated binary mixture in the framework of the homogeneous non-linear (Enskog-)Boltzmann equation for smooth inelastic hard spheres. Similarly to the case of free cooling described in and restricting to Gaussian velocity distributions, we derive in section II equations for the granular temperatures of the mixture components, which are easily solved numerically. The corresponding temperature ratio is in excellent agreement with existing numerical work. In section III, we consider the NESS sustained by heating through random kicks (“stochastic thermostat” approach), a mechanism which has focused some attention recently for one-component (monodisperse) systems. Although finding an energy injection mechanism of experimental relevance is a difficult issue, we expect the approach proposed here to elucidate the basic trends of grain behaviour when varying the controlling parameters. Moreover, as will be shown below, the temperature ratio we obtain provides a reasonable zeroth order approximation to compare with the experiments reported in.

II. KINETIC THEORY

We consider the model of smooth inelastic hard spheres (IHS) undergoing binary, momentum conserving, inelastic collisions, in the framework of the homogeneous non-linear Enskog equation. The system is a mixture of two types of...
IHS, with masses $m_1$ and $m_2$, diameters $\sigma_1$ and $\sigma_2$. Three types of collisions may occur so that the mixture is also characterized by three different restitution coefficients: $\alpha_{11}$, $\alpha_{22}$, and $\alpha_{12} = \alpha_{21}$.

The velocity distributions in the homogeneous state $f_i(v, t)$, $f_2(v, t)$, obey the following kinetic equations:

$$\partial_t f_i(v_1, t) = \sum_j J_{ij}[v_1|f_i, f_j] + \mathcal{F} f_i$$

(1)

where the $J_{ij}$ describe the effect of dissipative inter-particle collisions, and $\mathcal{F} f_i$ represents an external forcing which injects energy into the system, allowing it to reach a non-equilibrium steady state. The kernels $J_{ij}$ for collisions between a particle of type $i$ and a particle of type $j$ are given, in dimension $d$, by

$$J_{ij}[v_1|f_i, f_j] = \chi_{ij} \sigma_{ij}^{d-1} \int dv_2 \int d\tilde{\sigma} (\tilde{\sigma} \cdot v_{12}) \left( \frac{1}{\alpha_{ij}} f_i(v_1') f_j(v_2') - f_i(v_1) f_j(v_2) \right).$$

(2)

where the $\chi_{ij}$ are the pair distribution functions at contact (a priori unknown, but becoming close to 1 in the limit of low densities); $\tilde{\sigma}$ is a unit vector directed from the center of the particle of type $i$ to the center of particle $j$ [separated at contact by $\sigma_{ij} = (\sigma_i + \sigma_j)/2$], and the prime on the integral is a shortcut for $\int \Theta(\tilde{\sigma} \cdot v_{12})$. Moreover, $v_{12} = v_1 - v_2$, and the pre-collisional velocities $v_1'$ and $v_2'$ are given in terms of the post-collisional velocities $v_1$ and $v_2$ by:

$$v_1' = v_1 - \mu_{ji}(1 + \alpha_{ij}^{-1})(\tilde{\sigma} \cdot v_{12})\tilde{\sigma}$$

(3)

$$v_2' = v_2 + \mu_{ji}(1 + \alpha_{ij}^{-1})(\tilde{\sigma} \cdot v_{12})\tilde{\sigma}$$

(4)

where $\mu_{ij} = m_j/(m_i + m_j)$, so that momentum is conserved but energy dissipated.

The partial granular temperatures are defined from the kinetic energies by

$$\frac{n_i d T_i(t)}{2} = \int dv \frac{m_i v^2}{2} f_i(v, t),$$

(5)

$$n_i = \int dv f_i(v, t)$$

being the number density of particles of type $i$ with a total temperature of the mixture

$$T = \frac{1}{n_1 + n_2} \sum_i n_i T_i.$$  

(6)

From (1), the evolution equation for the temperatures reads

$$\partial_t T_i = \frac{m_i}{n_i d} \sum_j \int dv v^2 J_{ij}[v|f_i, f_j] + \mathcal{F} T_i,$$

(7)

where $\mathcal{F} T_i$ describes the effect of the forcing (source) term $\mathcal{F} f_i$. It is possible to integrate over $\tilde{\sigma}$ (see calculations in the appendix, and also [3]) to obtain, without any further approximation at this stage:

$$\partial_t T_i = \mathcal{F} T_i - \frac{\beta_3 m_i \chi_{ij} d_i \sigma_{ij}^{d-1}(1 - \alpha_{ij}^2)}{4n_i d} \int dv_1 dv_2 v_i^2 v_j^2 f_i(v_1) f_j(v_2)$$

$$- \frac{\beta_3 m_i \chi_{ij} d_i \sigma_{ij}^{d-1}}{n_i d} \int dv_1 dv_2 f_i(v_1) f_j(v_2) \left[ \mu_{ji}^2 (1 - \alpha_{ij}^2) v_{12}^2 + 2\mu_{ji}(1 + \alpha_{ij}) v_{12}(v_{12} \cdot V_{ij}) \right]$$

(8)

with $\beta_3 = \pi^{(d-1)/2}/\Gamma[(d + 3)/2]$, $V_{ij} = \mu_{ij} v_1 + \mu_{ji} v_2$, and $\Gamma$ the Euler function.

Since the system reaches a stationary state where the forcing term balances the dissipation due to collisions (the forcing and dissipative terms in (8) generically involve different powers of the temperatures so that its right-hand-side admits a “physical” root), we can write $\partial_t T_i = 0$. It is moreover convenient to scale the velocities with the thermal velocities $v_{0,i} = \sqrt{2 T_i/m_i}$, and introduce the functions $\Phi_i$ such that

$$f_i(v) = \frac{n_i}{v_{0,i}^d} \Phi_i \left( \frac{v}{v_{0,i}} \right).$$

(9)

Equation (8) may then be cast into an equation for the rescaled velocity distributions $\Phi_i$; no further step can however be taken without some approximations on the unknown distributions $\Phi_i$. It is convenient to study the deviations of $\Phi_i$ from the Gaussian $\Phi^0_i(c)$ through an expansion in Sonine polynomials [3]. In single component heated systems, the
deviation from a Gaussian remains small, especially for experimentally relevant values of the restitution coefficient $\alpha$. We will here limit our treatment to the Gaussian approximation $\Phi_1(c) = \Phi_0(c) = \exp(-c^2)$ (lowest order Sonine expansion). It would of course be possible to go further in a systematic and controlled way, as in [3], but we will see by comparison of our approximate analytical calculations with Monte Carlo simulations that, at least in the cases we consider, the Gaussian approximation provides reliable results.

Assuming Gaussian velocity distributions, it is now possible to carry out the remaining integrations in (8); the resulting equations for the granular temperatures $T_i$ in the NESS:

$$\frac{d\Gamma^d}{m_i\pi^{d-1}/2} \mathcal{F}T_i = \chi_{ii} \sigma_{ii}^{-1} n_i 2(1-\alpha_i^2)_{1/2} T_i^{3/2} + \chi_{ij} \sigma_{ij}^{-1} n_j \mu_{ji} \left[ \mu_{ji}(1-\alpha_j^2) \left( \frac{2T_i}{m_i} + \frac{2T_j}{m_j} \right) + 4(1+\alpha_{ij}) \frac{T_i - T_j}{m_1 + m_2} \right]^1 \right]. \tag{10}$$

These equations still depend on the particular heating mechanism through the term $F_T$; once the latter has been specified, two equations are obtained for $T_1$ and $T_2$; they are easy to implement and solve numerically varying the various controlling parameters.

Before turning to the heating provided by a stochastic thermostat [which amounts to $(F_T/m_i = constant)$, we consider three particular limiting cases.

a. In the tracer limit [13], i.e. $n_1 \to 0$, without any forcing term, $T_2$ is imposed and only the equation for $T_1$ is considered. As already noted in [3], the result for $\gamma = T_1/T_2$ obtained in [3]

$$\gamma = \frac{1 + \alpha_{12}}{2 + \frac{m_2}{m_1}(1 - \alpha_{12})} \tag{11}$$

is easily recovered, irrespective of dimension.

b. Another possibility to obtain a NESS for IHS has been proposed in [11]: the temperature $T_2 = T$ of one population is imposed, with a corresponding Gaussian velocity distribution, and elastic collisions between particles of type 2 as well as for $1 - 2$ collisions: $\alpha_{22} = \alpha_{12} = 1$. Energy is consequently injected into the inelastic population 1 (with restitution coefficient $\alpha_{11} = \alpha < 1$), without the need for any other forcing term. In [11], high precision numerical results were obtained for the distribution function $\Phi_1$, and temperature $T_1$ (the system is three-dimensional, and $\chi_{ij} = 1$), by an iterative numerical resolution of the Boltzmann equation. Imposing $F_T = 0$ in [11], it is straightforward to obtain a third order polynomial equation for $\gamma = T_1/T_2$ (this quantity is necessarily smaller than 1)

$$\frac{\varepsilon^2(1-\alpha^2)^2}{32} \left( \frac{m_1}{m_2} + \frac{m_2}{m_1} + 2 \right) \gamma^3 = (1-\gamma)^2 \left( \gamma + \frac{m_1}{m_2} \right) \quad \text{where} \quad \varepsilon = \frac{4n_1}{n_2(1+\sigma_2/\sigma_1)^2}. \tag{12}$$

In Fig. 1 the solution of equation (12) is compared to the results reported in [11]. The agreement is excellent, which may be traced back to the analysis of [11], showing that the distribution function $\Phi_1$ is very close to a Gaussian, although mathematically different (on the other hand and by definition of the model, $\Phi_2$ is strictly speaking a Gaussian). The slight discrepancy obtained at low $\alpha$ for $m_1 = m_2$ corresponds to values of the parameters for which the deviation of $\Phi_1$ from a Gaussian is stronger.

FIG. 1: Comparison of the simulation results found in [11] (lines) with the solution of equation (12) (circles), for various values of the mass ratio and of the parameter $\varepsilon$ recalled in (13).
Finally, a forcing term \( \mathcal{F} f_i(v) = \zeta \beta \cdot [v f_i(v)] \), which provides an Enskog-Boltzmann equation formally equivalent to the free cooling case (see e.g. [18]), leads back to the results of [8] obtained in this situation: the term \( \mathcal{F} T_i \) is indeed proportional to \( T_i \), so that writing \( \partial_t T_i = 0 \) in [8] yields the same equation for \( \gamma \) as equating the two cooling rates \( \partial_t T_i/T_i \) when \( \mathcal{F} T_i = 0 \).

## III. THE STOCHASTIC THERMOSTAT

In this section, we consider the situation of energy supply through random kicks [14, 15, 16, 17, 18, 19, 20, 21, 22]: the particles are submitted between collisions to an uncorrelated white noise (e.g. Gaussian). The equation of motion for a particle is then

\[
\frac{d v_i}{d t} = F_i + m_i \xi_i,
\]

where \( F_i \) is the force due to inelastic collisions, and \( \langle \xi_{i\alpha}(t)\xi_{j\beta}(t') \rangle = \xi_0^2 \delta_{ij} \delta_{\alpha\beta} \delta(t - t') \), where Greek indices refer to Cartesian coordinates. The associated forcing term in the Enskog equation is

\[
\mathcal{F} f = \frac{\xi_0^2}{2} \left( \frac{\partial}{\partial v} \right)^2 f(v, t),
\]

so that \( \mathcal{F} T_i = m_i \xi_0^2 \). We do not claim that the forcing term considered here is the most suited to describe vibro-fluidized beds, but it mimics an important effect of energy injection by a moving piston: in experiments, particles undergoing collisions with the piston (of large mass) gain a velocity that is decorrelated from their masses, so that more kinetic energy is injected into the population of large mass.

The corresponding equation for \( \gamma = T_1/T_2 \) reads:

\[
\chi_{11} \sigma_{11}^{-1} (1 - \alpha_{11}^2) n_1 \left( \frac{m_2}{m_1} \right)^{3/2} \gamma^{3/2} + \sqrt{2} \chi_{12} \sigma_{12}^{-1} \left[ (1 - \alpha_{12}^2) \left( \frac{m_2}{m_2} - \frac{n_1}{n_2} \gamma^2 \right) \left( 1 + \frac{m_2}{m_1} \gamma \right)^{3/2} \right. \\
\left. + 2 \mu_{21} (1 + \alpha_{12}) \left( \frac{m_2}{m_2} + \frac{n_1}{n_2} \gamma \right) \left( 1 + \frac{m_2}{m_1} \gamma \right)^{1/2} \right] = \chi_{22} \sigma_{22}^{-1} (1 - \alpha_{22}^2).
\]

The temperature ratio \( \gamma \) therefore depends in a non-trivial way on the ratios of masses, densities and diameters, and also on the inelasticities \( \alpha_{ij} \) and pair correlation functions \( \chi_{ij} \). It may be checked that in the limit of vanishing inelasticities, \( \gamma \rightarrow 1 \) as it should. Moreover, for mechanically equivalent particles (i.e. \( m_1 = m_2, \sigma_1 = \sigma_2 \) and \( \alpha_{11} = \alpha_{22} = \alpha_{12} \)), we should also recover equipartition (\( \gamma = 1 \)) irrespective of densities. This is the case in the Boltzmann limit (low densities where all pair correlation functions \( \chi_{ij} \rightarrow 1 \)). At arbitrary packing fraction, the various approximation for the \( \chi_{ij} \) that may be found in the literature [24, 25] are such that \( \chi_{ij} \) no longer depends on \( i \) and \( j \) when \( \sigma_1 = \sigma_2 \), so that equipartition holds for mechanically equivalent particles.

Since equation (14) relies on a Gaussian approximation for \( \Phi_0 \), we have compared our approach to the results of Monte Carlo simulations (the so-called DSMC technique [26]) where the non-linear Boltzmann equation is solved numerically for both species. As we solve numerically the homogeneous Boltzmann equation, the phenomena of segregation or clustering are explicitly discarded.

In the following sections, we will study more precisely some cases that could have experimental relevance, and for the sake of simplicity, we considered \( \chi_{ij} = 1 \). All the results are given for the three dimensional case; note however that for \( \sigma_1 = \sigma_2 \) the temperature ratio becomes \( d \)-independent.

### A. Equal inelasticities: \( \alpha_{ij} = \alpha \)

We first consider the case of equal restitution coefficients (\( \alpha_{ij} = \alpha \)), for materials having similar elastic properties. The dependence of \( \gamma \) on the mass and number density ratios, for equal sizes, is shown in Figure 2. Excellent agreement is found between DSMC simulations (symbols) and the solution of equation (14). It turns out indeed that the velocity distributions measured in Monte Carlo simulations are very close to Gaussians. As may be expected, \( \gamma \) is a decreasing function of \( m_2/m_1 \). The density dependence is relatively weak (the temperature ratio slightly increases when \( n_2/n_1 \) increases by an order of magnitude).

We have also considered two types of beads of the same material, i.e. the same restitution coefficient \( \alpha_{11} = \alpha_{22} = \alpha_{12} \) and same mass density \( \rho \): the ratio of masses \( m_2/m_1 \) is then equal to \( (\sigma_2/\sigma_1)^3 \) for three-dimensional beads. Figure
FIG. 2: Temperature ratio $\gamma = T_1/T_2$ as a function of inelasticity, for $\alpha_{11} = \alpha_{22} = \alpha_{12} = \alpha$, and grains of equal radii ($\sigma_1 = \sigma_2$). The curves show the solutions of equation (14) whereas the symbols display the results of DSMC simulations. The top three curves correspond to a mass ratio $m_2/m_1 = 2$, the three intermediate ones to $m_2/m_1 = 3$ and $m_2/m_1 = 5$ for the three bottom curves. For each mass ratio, several density ratios have been considered: $n_2/n_1 = 3$ (squares and dashed lines), $n_2/n_1 = 1$ (pluses and continuous lines), and $n_2/n_1 = 1/3$ (circles and dot-dashed lines).

shows a strong influence of the size ratio, for two experimentally relevant values of $\alpha$: $\gamma$ decreases very strongly as soon as $\sigma_2$ is two or three times $\sigma_1$. Once again, the number density ratio has a relatively small incidence on $\gamma$. It is interesting to disentangle the effects of $\sigma_2/\sigma_1$ and $m_2/m_1$, by varying one parameter alone, the other being kept constant. It appears that the leading effect in the decrease of $\gamma$ observed in Figure 2 is ascribable to a change in mass ratio, and not in size: the results obtained at $\sigma_1 = \sigma_2$ varying $m_2/m_1$ are close to those reported in Fig. 2, but surprisingly give a lower $\gamma$ (e.g. the results displayed in Figure 2 for $\alpha = 0.9$ and equal densities are $\gamma = 0.66$ and 0.38 for $\sigma_2/\sigma_1 = 2$ and 3 respectively, whereas with $\sigma_1 = \sigma_2$, we obtain $\gamma = 0.59$ for $m_2/m_1 = 2^3$ and $\gamma = 0.29$ for $m_2/m_1 = 3^3$).

FIG. 3: Temperature ratio from eq (14) for grains made of the same material, i.e. for $m_2/m_1 = (\sigma_2/\sigma_1)^3$, and $\alpha_{ij} = \alpha$. Filled symbols correspond to $\alpha = 0.9$, open ones to $\alpha = 0.7$. The squares are for $n_2/n_1 = 3$, the circles for $n_2/n_1 = 1$ and the diamonds for $n_2/n_1 = 1/3$.

B. Comparison with experiments

For glass spheres with size ratio $\sigma_2/\sigma_1 = 1.25$, Wildman and Parker have measured a temperature ratio $\gamma = T_1/T_2$ in the range 0.75-0.8 [6], with a weak dependence on densities (except may be in the limit of large grains predominance where $n_2 \gg n_1$). Estimating the relevant restitution coefficient to be $\alpha \simeq 0.9$ [6], we obtain from Eq. (14) $\gamma \simeq 0.9$ (see also Fig. 2), with also a weak dependence on $n_2/n_1$. It is however noteworthy that this weak dependence is opposite to that observed experimentally: when the proportion of large grains is increased, we obtain an increase of $\gamma$. For comparison, the temperature ratio obtained for the same parameters in the homogeneous cooling stage [8] is $\gamma \simeq 0.96$ and the authors of [8] proposed a simplified theory for which $\gamma$ is in the range 0.4-0.7.
The results obtained by Feitosa and Menon confirm the very weak influence of \( n_2/n_1 \) when the grains (of equal size) are made of two different materials. For a mixture glass/aluminum with mass ratio \( m_2/m_1 = 1.09 \), \( \gamma \) is measured very close to 1, whereas for a more asymmetric mixture of glass and brass with \( m_2/m_1 \approx 3.6 \), \( \gamma \approx 0.7 \). Making use of equation (14) with schematic inelasticities \( \alpha_{ij} = 0.85 \), we obtain \( \gamma = 0.98 \) for \( m_2/m_1 = 1.09 \) and \( \gamma = 0.7 \) for \( m_2/m_1 = 3.6 \). In the free cooling regime, the corresponding ratios are 0.99 and 0.82. These results are displayed in Fig. 4.

Other results are given in Figures 5 and 6 where the partial inelasticities are not taken equal, but are given values that we expect to be of experimental relevance: the experimental data of [7] are therefore also reported in Fig. 4(b). In Fig. 5, the sizes of the particles are taken equal and the mass ratio changes, while Fig. 6 displays the influence of the size ratio when the density ratios are fixed.

The situation reported in [7] corresponds to that of the Figures 5b and 6b, where the heavier grains are also the more dissipative. As may be observed in Fig. 5b, a variation of \( n_1/n_2 \) from 1/3 to 3 leaves \( \gamma \) roughly unaffected for \( m_2/m_1 \leq 3 \).

IV. CONCLUSION

We have considered heated binary granular mixtures from the point of view of kinetic theory. As in the free cooling case, and in agreement with recent experimental data, the granular temperatures of the components of the
readily computed and yields:

To compute the term containing $(\hat{\sigma} \cdot \nu)$, we choose one of the unit vectors to be along $\nu_{12}$, and decompose:

\[
\nu_{12} = \nu_{12} \hat{e}_1, \quad \nu = \frac{\nu_{12} \cdot \hat{e}_1}{\nu_{12}} + \nu_{12}^\perp, \quad \hat{\sigma} = \frac{\nu_{12} \cdot \hat{e}_1}{\nu_{12}} + \hat{\sigma}^\perp.
\]  

\[(\hat{\sigma} \cdot \nu)\] is then written as

\[
\frac{(\nu \cdot \nu_{12})(\hat{\sigma} \cdot \nu_{12})}{\nu_{12}^2} + \hat{\sigma}^\perp \cdot \nu_{12}^\perp,
\]
and the term $\hat{\sigma} \cdot v_1^\perp$ gives a vanishing contribution in the integral over $\hat{\sigma}$ for symmetry reasons. We are therefore left with

$$
\int d\hat{\sigma} \frac{(v_1 \cdot v_{12})(\hat{\sigma} \cdot v_{12})^3}{v_{12}^3} = v_{12}(v_1 \cdot v_{12}).
$$

Rearranging terms and writing $v_1 = \mu_{ji} v_{12} + \mu_{ij} v_1 + \mu_{ji} v_2 = \mu_{ji} v_{12} + V_{ij}$, one finally obtains equation (8).

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