Velocity fluctuations of a piston confining a vibrated granular gas

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Abstract. The steady state velocity fluctuations of a movable piston located on the top of a vibrated granular gas are studied by means of molecular dynamics simulations. From the second moment of the distribution, a temperature parameter for the piston is defined and compared with the granular temperature of the gas located just below it. Then the two temperature parameters refer to two interacting macroscopic systems. The equipartition of energy valid in usual molecular systems is strongly violated and the temperature of the piston can be larger or smaller than that of the gas, depending on the parameters defining the system at the particle level. The simulation results for the ratio of temperatures are in agreement with some theoretical predictions from kinetic theory, assuming the validity of a hydrodynamic description in the limit of weak inelasticity of the gas.
One of the characteristic features exhibited by granular fluids is the violation of the energy equipartition theorem. The granular temperatures of each of the components of a mixture, defined from the average kinetic energies of the particles, are not the same. This was pointed out long ago [1] and has attracted a lot of attention in the last decade or so. It is important to stress that the equality of the temperatures of the components of a mixture of molecular fluids is not restricted to equilibrium thermal systems, but also applies to out-of-equilibrium situations, at least to those that can be described by means of usual hydrodynamics as derived from kinetic theory or non-equilibrium statistical mechanics.

For the homogeneous cooling state (HCS) of a binary granular mixture modeled as an ensemble of smooth inelastic hard spheres, the ratio of temperatures of the two components has been obtained from an approximated solution of the kinetic Enskog equations [2]. This result is in good agreement with molecular dynamics (MD) simulation data [3]. The HCS is an idealized state in which the system cools homogeneously and monotonically. In real experiments, to maintain a fluidized granular system, external energy must be continuously supplied, and this is achieved by means of vibrating or rotating walls, by shearing, by shaking, or by other external fields. As a consequence, the systems become inhomogeneous. The non-equipartition has been confirmed by MD simulations of simple shear flows [4], and of vibrated gases [5, 6]. There are also some experimental evidence of the coexistence of different component temperatures in strongly vibrated granular mixtures [7, 8]. Homogeneously driven granular fluids submitted to stochastic forces have also been considered. The lack of energy equipartition in these systems has been analyzed [9], but the relationship between this kind of ideal driving and actual experiments is uncertain.

A peculiarity of the above studies is that they are concerned with quantities going beyond the macroscopic description, in the sense that the relevant macroscopic local property is the global temperature (or energy density) of the mixture, and not that of each of the components. Moreover, the latter are rather difficult to measure experimentally. Here, a possible experimental set-up in which the breakdown of energy equipartition is macroscopically observed is described and studied by means of MD and kinetic theory. The experiment is specifically designed to be reproducible in the laboratory and might have some practical advantages over previous related experiments [10], although it must be stressed that the study reported here is restricted to low density gases and that no friction between the particles, of the particles with the piston, or of the latter with the walls of the container is taken into account.

Consider a granular system composed of $N$ inelastic hard spheres ($d = 3$) or discs ($d = 2$) of mass $m$ and diameter $\sigma$. There is an external gravitational field acting on the system, so that each particle is subjected to a force $-mg_0\hat{e}_z$, where $g_0$ is a positive constant and $\hat{e}_z$ is the unit vector in the direction of the positive $z$ axis. The system is kept fluidized by vibrating the lower wall of the container in a sawtooth way, with very high frequency, negligible amplitude and velocity $v_W = v_W\hat{e}_z$ [11, 12]. The latter will be always taken large enough so as to keep the density of the system small everywhere. On the top of the system there is a movable lid or piston of mass $M$, as illustrated in figure 1. The piston can only move in the $z$ direction, remaining always perpendicular to it. It is assumed that there is no friction between the piston and the lateral walls of the vessel containing the granular gas.
Collisions between particles are inelastic and characterized by a constant coefficient of normal restitution \( \alpha \), so that when a pair of particles \( i \) and \( j \) collides, their relative velocity \( v_{ij} \) changes instantaneously according to

\[
v_{ij} \rightarrow v'_{ij} = v_{ij} - (1 + \alpha) \hat{\sigma} \cdot v_{ij} \hat{\sigma},
\]

(1)
while the total momentum is conserved. In the above expression, \( \hat{\sigma} \) is a unit vector directed from the center of particle \( j \) to the center of particle \( i \) at contact. Collisions of particles with the piston are also modeled as smooth and inelastic, \( \alpha_P \) being the coefficient of restitution in this case. Taking into account that the piston can only move in the \( z \) direction, the change in the relative velocity in a collision is restricted to the \( z \) component, and it is given by

\[
v_z - V_z \rightarrow v'_z - V'_z = v_z - V_z - (1 + \alpha_P)(v_z - V_z),
\]

(2)
where \( V_z \) is the velocity of the piston. This relation and the total momentum conservation define the collisions with the piston.

Next, some results from MD simulations of two-dimensional systems will be presented. To avoid undesired effects, periodic boundary conditions are used in the direction perpendicular to the external field. It is observed that, at least when the width \( W \) of the system is not too large, a steady state with no macroscopic flow of mass, and gradients in the fluid only in the direction of the external field, i.e. the \( z \) axis, is reached after some transitory period. This state is independent of the value of \( W \), as long as it is kept small enough. The shape of the hydrodynamic profiles in the bulk will be analyzed elsewhere [14], while here the emphasis will be put on the relationship between the temperature parameters of the piston, \( T_P \), and of the gas in its vicinity, \( T_G \). Both temperatures are defined from the second moment of the respective velocity distributions, namely \( M\langle v_z^2 \rangle \equiv T_P \), \( m\langle v^2 \rangle \equiv 2T_G \), with the angular brackets denoting average. In the results to be reported in the following, units defined by \( m = 1 \), \( \sigma = 1 \) and \( g_0 = 1 \) will be used.
Figure 2. Steady velocity distribution of the piston $P(V_z)$ in both logarithmic and normal scales. The symbols are from MD simulations while the solid line is a Gaussian fitting. The values of the parameters defining the system and the dimensionless unit for the velocity $V_z$ are given in the main text.

The measured probability distribution for the velocity of the piston is very well fitted by a Gaussian in all the cases considered. A typical example, corresponding to $v_W = 11$, $\alpha = 0.9$, $\omega_P = 1$, $M = 49$, $N = 420$ and $W = 70$, is given in figure 2. For this case, the value $T_P \simeq 58.67$ is found. It is seen that the Gaussian fit is accurate at least up to values of the probability density of the order of $10^{-4}$. The measurement of $T_G$ is somewhat more problematic, since the ‘top region’ of the granular gas next to the piston has to be identified. Here, the layer of the gas defined by $\langle Z \rangle - 2\sigma_Z \leq z \leq \langle Z \rangle + 2\sigma_Z$, where $\sigma_Z$ is the dispersion of the values of the position of the piston $Z$, has been used. Then, the average over the velocities to compute $T_G$ has been carried out over the particles inside this region at each time. This criterion may appear as rather arbitrary, but it has been checked that other sensible choices, such as extrapolating the bulk temperature profile to $\langle Z \rangle$, lead to values of the temperature with discrepancies of the order of 5%. In this way, it is found that $T_G \simeq 37.69$, implying $T_P/T_G \simeq 1.56$. This represents a strong violation of the energy equipartition, especially taking into account that the collisions between the grains and the piston have been modeled as elastic ($\alpha_P = 1$). Moreover, it must be stressed that the temperature parameter of the piston is larger than the temperature of the gas transmitting to it the effects of the lower vibrating wall. It can be wondered whether this effect is related to some strong anisotropy of the velocity distribution of the gas. Let us define $T_{Gx} \equiv m\langle v_x^2 \rangle$ and $T_{Gz} \equiv m\langle v_z^2 \rangle$, so that $T_G = (T_{Gx} + T_{Gz})/2$. Then, for the particular case we are discussing, it is found that $T_{Gz}/T_{Gx} \simeq 1.096$. Therefore, although there is some anisotropy as usual in vibrated granular systems, it is very weak as compared with the excess value of $T_P/T_G$. More precisely, it is $T_P/T_{Gz} \simeq 1.49$. The
same trend is observed in all the other cases investigated, being the given above the one in which the anisotropy of the second moment of the velocity tensor is stronger.

In figure 3, the temperature ratio $T_P/T_G$ is plotted as a function of the coefficient of restitution of the gas $\alpha$ for three different values of the pair $(M, \alpha_P)$, illustrating the influence of each of these parameters on the temperature ratio. Quite interestingly, the violation of equipartition (deviation of the temperature ratio from unity) is not a monotonic function of $\alpha$, but the temperature ratio exhibits a minimum in the small inelasticity region. The result with $\alpha = 1, \alpha_P = 1$, has been obtained with a non-vibrated system at thermal equilibrium. As expected, equipartition is recovered in the limit $\alpha = \alpha_P = 1$. The reason to restrict the analysis to the inelasticity region $\alpha \geq 0.9$ is that, for smaller values, even the hydrodynamic description of the bulk of the gas, as provided by the Navier–Stokes equations, breaks down [14].

An expression for the temperature ratio can be derived as follows. Given the low density of the gas, a pair of coupled Boltzmann and Boltzmann–Lorentz kinetic equations are used as the starting point to describe both the gas and the piston. The subsequent calculations are based on the following two assumptions: (a) the macroscopic state of the piston can be specified in terms of the hydrodynamic fields of the gas in its vicinity and its position probability distribution and (b) the associated normal solution of the kinetic equations can be generated by the Chapman–Enskog procedure. With these hypotheses, it is obtained that the zeroth order in the gradient cooling rates of the piston, $\zeta_P^{(0)}$, and of the top region of the gas, $\zeta_G^{(0)}$, must be the same [14,13]. These rates are functionals of the one-particle distributions for the top region of the fluid and the piston. Given that these distributions are not known, Maxwellians can be used as an estimation. Therefore, no anisotropy effects are introduced in the theory. A generalization of the derivation in [13], with the peculiarity that now all the collision vectors have the same direction,
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Figure 4. Ratio \( \phi \equiv mT_p/MT_G \) of the thermal velocities for the piston and the gas just below it. The lines are from equation (6) and the symbols are MD simulation results for hard discs.

leads to [14]

\[
\zeta_P^* \equiv \frac{\zeta_P^{(0)}}{n_G v_T \sigma^{d-1}} = \frac{4W_h}{\pi^{1/2} \sigma^{d-1}} \left(1 + \frac{\phi}{\phi} \right)^{1/2} \left(1 - h \frac{1 + \phi}{\phi} \right),
\] (3)

\[
\zeta_G^* \equiv \frac{\zeta_G^{(0)}}{n_G v_T \sigma^{d-1}} = \frac{\sqrt{2} \pi^{(d-1)/2}}{\Gamma(d/2)} d (1 - \alpha^2),
\] (4)

where \( n_G \) is the gas density in the top region, \( v_T \equiv (2T_G/m)^{1/2} \), \( \phi \equiv mT_p/MT_G \), and

\[
h \equiv \frac{m(1 + \alpha_P)}{2(m + M)}.
\] (5)

Note that all the dependence on the mass ratio and the inelasticity \( \alpha_P \) occurs through \( h \). Requiring the cooling rates to be the same, an equation determining \( \phi \) is obtained:

\[
h \left(1 + \phi\right)^{1/2} \left(1 - h \frac{1 + \phi}{\phi} \right) = \frac{(1 - \alpha^2) \pi^{d/2} \sigma^{d-1}}{2\sqrt{2} \Gamma(d/2) W d}.
\] (6)

The elastic collisions’ limit \( (\alpha = \alpha_P = 1) \) is given by \( \phi = h/(1 - h) = m/M \), that is the equipartition result. If the particle collisions are elastic but not those with the piston \( (\alpha = 1, \alpha_P < 1) \), it is \( \phi = m(1 + \alpha_P)/(2M + m(1 - \alpha_P)) \). This result is the same as the one derived in [15] for an inelastic intruder in an equilibrium elastic gas.

The prediction made by equation (6) is compared with some MD simulation results in figure 4, where \( \phi \) is plotted as a function of \( h \). In the simulations, the values of the latter quantity have been modified by changing both \( M \) (in the range 10–140) and \( \alpha_P \) (between 0.6 and 1). The other parameters \( (W, v_W, N) \) are kept the same as in figure 2. The symbols are the simulation results while the lines are from equation (6), as indicated. Data

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for two values of $\alpha$, 0.98 and 0.9, are reported. For the most elastic gas, the agreement is quite good, for all the considered values of the other parameters. Nevertheless, when the inelasticity of the gas is slightly increased, strong deviations from the theoretical prediction show up. These discrepancies are not only quantitative, but also qualitative. The circled symbols on the left lower corner of the figure correspond to $M = 49$, differing in the value of $\alpha_F$. It is observed that, when $\alpha_F$ (and $h$) increases, $\phi$ decreases, in contradiction to the solution of equation (6). To identify the cause of the failure of the theory, the shape of the marginal distribution of the component of the velocity of the grains perpendicular to the piston in the top region, $\varphi(v_z)$, has been measured. While for $\alpha = 0.98$ it is always well fitted by a Gaussian within the numerical error of the simulations, for $\alpha = 0.9$, exponential tails are clearly identified for positive velocities already in the thermal range, as is seen in figure 5. These tails are relevant for the lowest velocity moments of the gas. On the other hand, it was already mentioned above (see figure 2) that the velocity distribution of the piston remains Gaussian. A theoretical analysis of the existence of this exponential tail probably requires going beyond the Chapman–Enskog method, the restriction to normal solutions of the Boltzmann equation and, therefore, of the hydrodynamic description.

The above results seem to provide additional evidence of the difficulties when trying to give a macroscopic meaning to the granular temperature, at least as defined in kinetic theory and the usual hydrodynamic theories. The knowledge of the hydrodynamic profiles of the confined gas and the characteristics of the interactions between the gas particles and the piston is not enough to determine the ‘temperature’ of the latter. More detailed information about the velocity distribution of the gas in its vicinity is required. Moreover, it is surprising that sometimes the ‘temperature’ of the body to which energy is supplied (the piston) can be larger than the temperature of the system supplying the energy (the neighbor gas). The results also show that this effect is not associated with the
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Anisotropy of the gas. Finally, let us stress the differences of this system as compared with a gas mixture, even in the tracer (one-intruder) limit. Here, two macroscopic systems spatially differentiated are interacting on contact, their respective states being strongly interdependent. As a consequence, it seems clear that both temperature parameters have a macroscopic meaning.

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