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Abstract. A fluidized granular gas in presence of a gravitational field is considered. It is enclosed in a box with a movable piston on the top. Molecular dynamics simulation results show that, if the box is not too wide, the system reaches a stationary state with gradients only in the direction of the field. Here, attention is focussed on the velocity fluctuations of the piston, that are observed to be Gaussian. The relationship between the second moment of this distribution and the granular temperature of the gas just below it is investigated. The ratio between the mean square velocities of the pisto and the gas can be larger or smaller than unity depending on the parameters of the system. A kinetic theory is formulated and its predictions compared with the simulation data.

Keywords: granular gases, fluctuations, non-equilibrium temperature
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INTRODUCTION

Granular materials are ubiquitous in nature and fundamental to many industries, including the chemical, pharmaceutical, metallurgical, food, agricultural, and construction ones. They are collections of discrete macroscopic solid particles. Typically, the energy necessary to lift one grain of sand a height equal to its diameter exceeds at least by 12 orders of magnitud the thermal energy at room temperature. Also the kinetic energy of a grain moving with a typical velocity of 1 cm /sec is much larger than the typical thermal energy. Consequently, thermal fluctuations in the usual sense are not enough to move the grains and, therefore, play no role in the dynamics of these materials. Moreover, the forces between grains are inherently dissipative, i.e. mechanical energy is not conserved in the interactions. Because of the above reasons, the properties of granular materials are often quite different from those of molecular gases, liquids, and solids [1]. In the last two decades, there has been a renaissance in the interest of physicists in the study of granular systems. This has been prompted and stimulated by the results of a series of experiments using novel techniques and also by the realization that granular physics presents many theoretical challenges and offers a fascinating proving ground for fluid dynamics, theory of elasticity, nonequilibrium statistical mechanics, and many other domains of physics.

Due to the loss of energy in collisions, to maintain the grains in movement, energy has to be continuously supplied to the system from some external sources. When the latter are strong enough, the granular system can exhibit fluid-like behavior, although with significant differences as compared with molecular fluids. This is the so-called fast flow regime in which the grains can be considered to move independently between collisions [2, 3]. The methods of kinetic theory and non-equilibrium statistical mechanics have been extended to describe fast granular flows, often referred to as granular gases [4]. One

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of the main results obtained are generalized Navier-Stokes hydrodynamic equations. In the case of one-component systems with no rotational friction, they are closed equations for the number of particles density $n(\mathbf{r},t)$, the flow velocity $\mathbf{u}(\mathbf{r},t)$, and the *granular temperature*, $T(\mathbf{r},t)$. This latter field is defined either in terms of the second moment of the local velocity distribution of the gas or from the local total energy [5], without any thermodynamic-like meaning, at least in principle.

The simplest model of a mono-disperse granular fluid is a system composed of smooth, inelastic hard spheres ($d = 3$) or disks ($d = 2$) of mass m and diameter σ. Besides, there is no interstitial fluid. The only difference with the corresponding model for normal fluids is a loss of kinetic energy in each binary collision. This loss is characterized by a constant coefficient of normal restitution α, defined in the interval $0 < \alpha \leq 1$, with $\alpha = 1$ giving the elastic limit. Then, when two of these particles with velocities $\mathbf{v}_i$ and $\mathbf{v}_j$ collide, their velocities change instantaneously according with

$$\mathbf{v}_i \rightarrow \mathbf{v}'_i = \mathbf{v}_i - \frac{1+\alpha}{2}(\widehat{\sigma} \cdot \mathbf{v}_{ij})\widehat{\sigma}, \tag{1}$$

$$\mathbf{v}_i \rightarrow \mathbf{v}'_j = \mathbf{v}_i + \frac{1+\alpha}{2}(\widehat{\sigma} \cdot \mathbf{v}_{ij})\widehat{\sigma}, \tag{2}$$

where $\mathbf{v}_{ij} \equiv \mathbf{v}_i - \mathbf{v}_j$ is the relative velocity and $\widehat{\sigma}$ is the unit vector pointing from the center of particle j to the center of particle i at contact. This model has proven to lead to many of the peculiar qualitative behaviors exhibited by real granular gases [6, 7]. In the low density limit, the system can be described by means of the inelastic Boltzmann equation [8] for the one-particle distribution function. Assuming the existence of a normal solution, closed hydrodynamic equations have been derived using an extension of the Chapman-Enskog procedure [9, 10]. These are the (inelastic) Navier-Stokes equations mentioned above. Extensions to denser systems and also to granular mixtures have been carried out in the context of the (inelastic) Enskog equation [11].

In the above works and also in many others, attention has been focussed on kinetic equations for the one-particle distribution function and the derivation of hydrodynamic descriptions from those equations. Also, linear hydrodynamic equations valid for granular fluids of arbitrary density have been derived by means of linear response theory [5, 12]. On the other hand, the knowledge about correlations and fluctuations of the hydrodynamic fields in granular gases is much more limited. There has been some studies using the equations of molecular fluctuating hydrodynamics [13], and incorporating the effects of inelasticity just through the time dependence of the temperature and a new term involving the cooling rate in the equation for the energy [14, 15]. The purpose of these studies was to investigate the fluctuations and correlations in freely evolving granular gases under conditions such that the homogeneous cooling state (HCS) is unstable due to a hydrodynamic long wavelength instability leading to the formation of velocity vortices and density clustering [16, 17].

For dilute granular gases in the HCS, a general theory of fluctuations and correlations has been formulated [18], using the so-called hierarchical method [19]. The general idea behind this procedure is to start from the Liouville equation of the system and derive hierarchies of equations for the distributions functions describing equal and different time correlations. For practical applications, these hierarchies must be closed by means of some approximation. The nice point is that the same kind of hypothesis used to derive the corresponding kinetic equation, e.g. the Boltzmann equation, also suffices in this more general context [19]. In this way, both non-equilibrium averages and fluctuations are embodied in a unique scheme, similarly to what happens in equilibrium theory.

Here, a very simple situation will be considered, in order to identify some of the direct effects that inelasticity has over the velocity fluctuations, and the way they are transmitted from one system to another. A vibrated granular gas in presence of gravity is confined by means of a piston placed on top of it. As a consequence of the collisions of the grains with the piston, the latter exhibits an oscillatory motion. Under certain conditions, the system reaches a steady state in which the average position of the piston does not depend on time. Also its velocity distribution becomes stationary. Moreover, the simulation results shows that it is very accurately Gaussian. The issue addressed here is the relationship between the second moment of these steady velocity fluctuations of the piston and the velocity distribution of the gas generating them. For an elastic system with no external field, the gas is at equilibrium with the same temperature as the one defined from the velocity fluctuations of the piston. On the other hand, for vibrated inelastic gases, the mean square velocities of the piston and the neighbor gas can be rather different. Even more, their ratio can be larger or smaller than unity depending on the values of the parameters defining the system.

VELOCITY FLUCTUATIONS OF A PISTON CONFINING A FLUIDIZED GRANULAR GAS

Consider a collection of N inelastic hard spheres or disks in a box, in presence of gravity, being g the gravitational acceleration. To maintain the system fluidized, energy is continuously supplied by vibrating the wall located at the bottom. The results to be presented in the following are independent of the specific way in which the wall is vibrated, as long as the amplitude be sufficiently small and the frequency high enough. Also, the details of the collisions between this wall and the grains are expected to be irrelevant, at least in the case of monodisperse systems [20], which is the one considered here

Next, the upper boundary condition will be described. The case of an open system has been studied elsewhere [21], and it was shown that the hydrodynamic profiles predicted by the inelastic Navier-Stokes equations are in good agreement with particle simulation results, at least in the limit small inelasticity, i.e. for values of α close to unity. Here a rather different physical situation will be investigated. It will be considered that there is a movable lid or piston on top of the gas as illustrated in Fig. 1. The piston has a finite mass M and can only move in the direction of the gravitational field, taken as z-axis. There is no friction between the piston and the lateral walls of the vessel.

Collisions of particles with the piston are characterized by a constant coefficient of normal restitution α_P, so that when a particle with velocity $\mathbf{v}$ collides with the piston having the latter a velocity V_Z, their after-collision velocities are given by

$$v_z' = v_z - \frac{M}{m+M}(1+\alpha_P)(v_z - V_z), \tag{3}$$

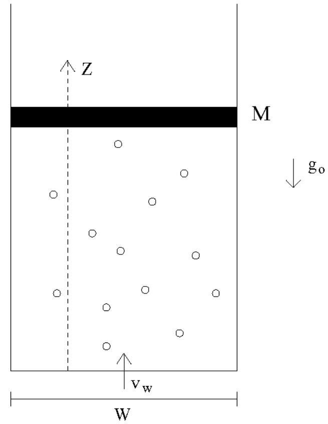

FIGURE 1. Sketch of the setup described in the text

$$V_z' = V_z + \frac{m}{m+M}(1+\alpha_P)(v_z - V_z), \tag{4}$$

the vector component of the velocity of the particle parallel to the piston remaining unchanged.

The behavior of the above system has been investigated by means of molecular dynamics (MD) simulations. In the following results for inelastic hard disks ($d = 2$) will be reported. To avoid undesired boundary effects, periodic boundary conditions are used in the direction parallel to the piston, substituting the lateral walls. If the width W is not too large, the system reaches a macroscopic stationary state without mass flow and with gradients of the fields in the fluid only in the direction of the external field. As an example, in Fig. 2 the steady temperature and density profiles obtained in a system with $\alpha = 0.96$, $M/m = 60$, and $\alpha_P = 1$ are plotted. The wall at the bottom was vibrated with a sawtooth velocity profile [22]. The steady hydrodynamic profiles only depend on W through the ratio $N\sigma/W$. The vertical dotted line in the figure indicates the average position of the piston. The plotted hydrodynamic profiles extend to values of z that are appreciably larger than this average position due to the rather large fluctuations of the piston. This behavior is exemplified in Fig. 3, where the time evolution of the height z of the piston once in the steady state is plotted for an arbitrary MD simulation trajectory. The system is the same as in Fig. 2 and steady average position of the piston is now indicated by the horizontal dashed line. The fluid temperature profile seems to monotonically decrease towards a constant value, although it actually exhibits a weak minimum [21, 23]. On the other hand, the density profile presents a maximum.

The hydrodynamic profiles measured in the simulations are in good agreement with theoretical predictions based on the hydrodynamic Navier-Stokes equations for a dilute gas of inelastic hard particles and the appropriate boundary conditions [23]. This issue will not be discussed here, but it is worth to point out that both the apparent plateau in the temperature profile and the decay of the density profile after its maximum lie well inside the hydrodynamic region, and not into the kinetic boundary layers. Moreover, the

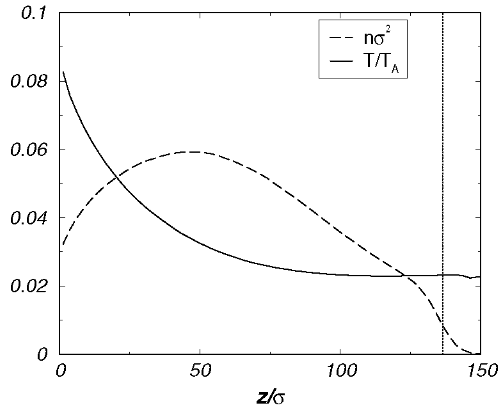

FIGURE 2. Temperature (solid line) and density (dashed line) profiles of a vibrated system with $\alpha = 0.96$, $\alpha_P = 1$, $M = 60m$, and $N\sigma/W = 6$. The temperature is scaled with an arbitrary reference value T_A, in order to fit it into the same scale as the density profile. The wall at the bottom moves in a sawtooth way with a velocity $v_W = 4\sqrt{g\sigma}$, very high frequency and vanishing amplitude.

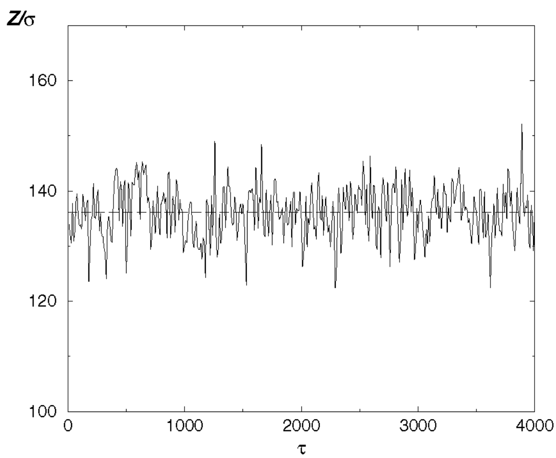

FIGURE 3. Time evolution of the position of the piston for the same system as in Fig. 2. Time is measured in accumulated number of collisions per particle.

density maximum is not associated to any clustering instability.

As mentioned above, the fluctuations of the piston around its average position in the steady state are quite large. Attention will be restricted here to its velocity fluctuations. Analysis of the simulation data shows that they are very well fitted by a Gaussian within the statistical uncertainties for all the cases investigated ($\alpha \geq 0.9$) [24]. Therefore, the velocity fluctuations of the piston can be characterized by means of the second moment of its probability distribution or, equivalently, by a temperature parameter T_P defined

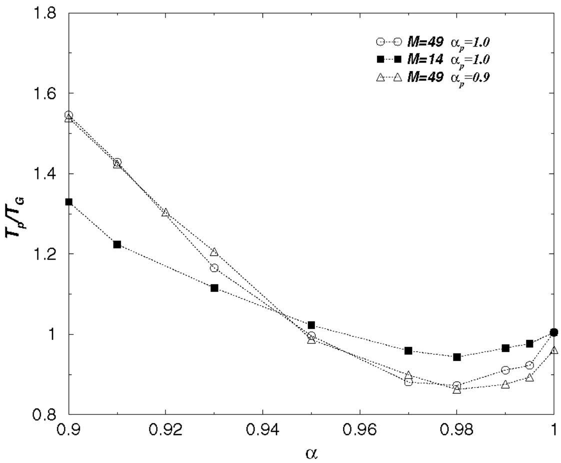

FIGURE 4. Temperature parameter of the piston T_P relative to the granular temperature of the gas in its vicinity T_G, as a function of the restitution coefficient of the gas α. The lines are just guides for the eye. The values of the mass M in the legend are given in units of m.

as $M < V_z^2 > \equiv T_P$, where the angular brackets denote average over the steady velocity distribution of the piston. Note that the Boltzmann constant factor k_B does not appear in the definition of T_P, as it is customary in the context of granular systems, to emphasize its lack of any thermodynamical meaning. It is interesting to compare the parameter T_P with the granular temperature of the gas in the vicinity of the piston, T_G, given by $m < v^2 >= 2T_G$. Now the average is taken over the velocity distribution of the gas in a narrow layer below the piston. Although there are several sensible choices to identify this layer, all of them lead to practically the same value of T_G [23].

In Fig. 4, the values of the ratio T_P/T_G obtained from MD simulations are plotted as a function of the coefficient of restitution of the gas α in the interval $0.9 \leq \alpha \leq 1$. Three series of data are reported, corresponding to different values of the coefficient of restitution for grain-piston collisions and/or the mass of the piston, namely ($\alpha_P = 1, M = 49m$), ($\alpha_P = 1, M = 14m$), and ($\alpha_P = 0.9, M = 49m$), respectively. The results in the elastic limit $\alpha = \alpha_P = 1$ have been obtained by keeping the bottom wall at rest and, therefore, refer to an equilibrium system in presence of gravity.

Several conclusions follow from inspection of Fig. 4. The first one is that both temperature parameters can be rather different, discrepancies larger than 50% being observed for the largest disparity of masses analyzed. A second conclusion is that the dependence of the temperature ratio on the several parameters of the system is quite involved. Monotonic behavior is not observed in any of them. Moreover, T_P/T_G is smaller than unity near the elastic gas limit, exhibiting a minimum roughly around $\alpha \approx 0.98$. When the coefficient of restitution α decreases further, the ratio of the temperature parameters T_P/T_G grows quite fast. It is also observed that the mass of the piston influences the temperature ratio much more than the inelasticity of the collisions between the particles and the piston. Actually, the curves corresponding to $\alpha_P = 1$ and

$\alpha_P = 0.9$, both with $M/m = 49$ are almost undistinguishable on the scale of the figure. It must be noticed that $\alpha_P = 0.9$ is already considered as a value characterizing rather inelastic collisions.

If T_P and T_G are interpreted as (non-equilibrium) temperatures of the gas and the piston, respectively, the results in Fig. 4 can be seen at first as a violation of the energy equipartition occurring in equilibrium systems. It is well known that the partial granular temperatures of each of the components of a mixture of grains are not the same [25, 26, 27, 28, 29]. This feature is quite well captured by the kinetic theory description of granular gas mixtures, the theoretical predictions being in good quantitative agreement with MD simulations. To put this into a proper conceptual context, it is important to stress that the granular temperatures of the components of the granular mixture are assumed to play no role in the macroscopic description of the mixture. The hydrodynamic equations governing the macroscopic evolution of the system only involve one temperature field, defined in the usual way from the average of the total local kinetic energy [26].

The situation being considered here is quite different. The temperature parameters T_G and T_P refer to two well differentiated macroscopic systems, namely the granular gas and the piston, occupying at every time different space regions. Both, T_P and T_G, can be easily measured from the respective velocity distributions. The "violation" of equipartition in this context must be understood as the difference in temperature parameters between two bodies which are at contact in a steady state. Of course, this difference is not at all surprising, since there is no reason to extend equilibrium properties to far from equilibrium situations. Nevertheless, what is somehow surprising is the very complicated relationship between T_P and T_G, as illustrated in Fig. 4. In particular, it does not seem easy to explain why in some parameter region, T_P is larger than T_G. If both quantities were associated when the usual concept of temperature, it would follow that a system (the gas) is heating another system (the piston) to a larger temperature than its own one. In a rough way, it could be said that the energy seems to flow in the "wrong" direction.

KINETIC THEORY

To determine the statistical properties of the velocity of the piston, its dynamics must be modeled. Consider the probability density $P(z,V_z,t)$ of finding the piston at a height z with a velocity V_Z at time t. If pre-collisional correlations between the velocity of the piston and those of the particles colliding with it are assumed to be negligible, the time evolution of $P(z,V_z,t)$ is described by the Boltzmann-Lorentz equation [30]

$$\left(\frac{\partial}{\partial t} + V_z \frac{\partial}{\partial z} - g \frac{\partial}{\partial V_z}\right) = J[z,V_z,t|P,f], \tag{5}$$

with the collision term J given by

$$\begin{aligned} J[z,V_z,t|P,f] \quad = \quad & W \int d\mathbf{v}\, |v_z - V_z| \left[\alpha_P^{-2} \theta(V_z - v_z) f(z,\mathbf{v}^*,t) P(z,V_z^*,t)\right. \\ & \left. -\theta(v_z - V_z) f(z,\mathbf{v},t) P(z,V_z,t)\right]. \end{aligned} \tag{6}$$

Here, $f(z,\mathbf{v},t)$ is the one-particle distribution of the gas. It is given by the solution of the nonlinear inelastic Boltzmann equation, the piston playing the role of a boundary condition [31]. For the sake of simplicity, attention is being restricted to states of the gas with gradients only in the direction of the external fields, so that f only depends on position through the z coordinate. This includes, in particular, the steady state discussed in the previous section. Moreover, θ is the Heaviside step function, and $\mathbf{v}^*$ and v_z^* are the so-called *restituting velocities*, i.e. the initial values of the velocities leading to $\mathbf{v}$ and V_z following the collision. By using Eqs. (3) and (4) they are seen to be given by

$$v_z^* = v_z - \frac{M}{m+M}\frac{1+\alpha_P}{\alpha_P}(v_z - V_z), \tag{7}$$

$$V_z' = V_z + \frac{m}{m+M}\frac{1+\alpha_P}{\alpha_P}(v_z - V_z), \tag{8}$$

the other components of $\mathbf{v}^*$ being the same as those of $\mathbf{v}$. The difference between the formal expressions for the post-collisional velocities, Eqs. (3) and (4), and those for the restituting ones, Eqs. (7) and (8), is a direct consequence of the inelasticity of collisions.

Now, it will be assumed that on the appropriate time and length scales, Eq. (5) as well as the Boltzmann equation for the gas have "normal" solutions, characterized because all the space and time dependence of the distribution functions occurs through the hydrodynamic fields of the gas, $n(\mathbf{r},t)$, $\mathbf{u}(\mathbf{r},t)$, $T(\mathbf{r},t)$, and, in the case of $P(z,V_z,t)$, the number density of the piston $\mathscr{N}$, defined by

$$\mathscr{N}(z,t) = \int dV_z P(z,V_z,t). \tag{9}$$

Also, in the spirit of the Chapman-Enskog algorithm [30, 32], it will be assumed that the normal solutions can be generated by expressing them as series expansions in powers of a formal non-uniformity parameter ε [31],

$$P(z,V_z,t) = P^{(0)}(z,V_z,t) + \varepsilon P^{(1)}(z,V_z,t) + \varepsilon^2 P^{(2)}(z,V_z,t) + \ldots, \tag{10}$$

$$f(z,\mathbf{v},t) = f^{(0)}(z,\mathbf{v},t) + \varepsilon f^{(1)}(z,\mathbf{v},t) + \varepsilon^{(2)} f^{(2)}(z,\mathbf{v},t) + \ldots, \tag{11}$$

where each factor of ε means an implicit gradient of a macroscopic field. The above expansions imply a corresponding expansion of the formal expressions of the pressure tensor, the heat flux, and the cooling rates. In addition, the time derivatives of the fields are also expanded in powers of ε,

$$\partial_t = \partial_t^{(0)} + \varepsilon \partial_t^{(2)} + \varepsilon^2 \partial_t^{(2)} + \ldots, \tag{12}$$

by means of the balance equations [30]. Thus to lowest order it is found

$$\partial_t^{(0)} n = \partial_t^{(0)} \mathbf{u} = \partial_t^{(0)} \mathscr{N} = 0, \tag{13}$$

$$\partial_t^{(0)} T = -\zeta^{(0)} T, \tag{14}$$

with $\zeta^{(0)}$ being the lowest order in the gradients of the cooling rate of the gas [9]. The leading order of Eq. (5) reads

$$-\zeta^{(0)}T\frac{\partial}{\partial T}P^{(0)}=J[z,V_z,t|P^{(0)},f^{(0)}], \tag{15}$$

where the zeroth order in ε distribution function of the gas $f^{(0)}$ is that of a *local* homogeneous cooling state, having the scaling form [8, 9]

$$f^{(0)}(z,\mathbf{v},t)=nv_T^{-1}\varphi\left(\frac{c}{v_T}\right), \tag{16}$$

where

$$v_T(z,t)=\left[\frac{2T(z,t)}{m}\right]^{1/2} \tag{17}$$

is a local thermal velocity and φ an isotropic function of the peculiar velocity $\mathbf{c}(z,t)=\mathbf{v}-\mathbf{u}(z,t)$. Then, dimensional analysis requires that

$$P^{(0)}(z,V_z,t)=\mathscr{N}v_T^{-1}\chi\left(\frac{C_z}{v_T}\right), \tag{18}$$

being also χ an isotropic function of its argument, $C_z(z,t)=V_z-u_z(z,t)$. As a consequence, Eq. (15) is equivalent to

$$-\frac{\zeta^{(0)}}{2}\frac{\partial}{\partial C_z}\left(C_zP^{(0)}\right)=J[z,V_z,t|P^{(0)},f^{(0)}]. \tag{19}$$

.

Multiplication of this equation by MC_z^2 and integration over V_z yields

$$\zeta^{(0)}(z,t)=\zeta_P^{(0)}(z,t) \tag{20}$$

where

$$\zeta_P^{(0)}(z,t)\equiv-\frac{M}{\mathscr{N}(z,t)T_P(z,t)}\int_{-\infty}^{\infty}dC_zC_z^2J\left[z,V_z,t|P^{(0)},f^{(0)}\right] \tag{21}$$

is the cooling rate for the temperature parameter of the piston T_P as defined in the previous section. Upon deriven Eq. (20) it has been taken into account that in the Chapman-Enskog procedure it is

$$\int dV_zC_z^2P(z,V_z,t)=\int dV_zC_z^2P^{(0)}(z,V_z,t), \tag{22}$$

as required by the solubility conditions of the equations generated by the expansion in powers of ε of Eq. (5) [33].

The evaluation of the cooling rates $\zeta^{(0)}$ and $\zeta_P^{(0)}$ requires to solve the equation for $f^{(0)}(z,\mathbf{v},t)$ and, afterwards, Eq. (19). This can be done in a systematic way by expanding

$f^{(0)}$ and $P^{(0)}$ in terms of an ensemble of orthogonal polynomials [26]. Here we will consider a leading order approximation that is expected to give quite accurate results, at least for not very strong inelasticity. The zeroth order distributions are approximated by Gaussians,

$$f^{(0)}(z,\mathbf{v},t) = n\left(\frac{m}{2\pi T_G}\right)^{d/2} e^{-mv^2/2T_G}, \tag{23}$$

$$P^{(0)}(z,V_z,t) = \mathcal{N}\left(\frac{M}{2\pi T_P}\right)^{1/2} e^{-MV_z^2/2T_P}. \tag{24}$$

Note that the latter expression is consistent with the condition given by Eq. (22) if T_P is identified with the actual temperature parameter of the piston as defined in the previous section and measured by means of MD simulations. Employing Eqs. (23) and (24), it is straightforward to calculate the cooling rates. The technical details are similar to those discussed, for instance, in [26] and [34] and will be not reproduced here. The result is

$$\zeta_P^* \equiv \frac{\zeta_P^{(0)}}{nv_T\sigma^{d-1}} = \frac{4Wh}{\pi^{1/2}\sigma^{d-1}}(1+\phi)^{1/2}\left(1-h\frac{1+\phi}{\phi}\right), \tag{25}$$

$$\zeta^* \equiv \frac{\zeta^{(0)}}{nv_T\sigma^{d-1}} = \frac{\sqrt{2}\pi^{(d-1)/2}}{\Gamma(d/2)d}(1-\alpha^2), \tag{26}$$

where

$$\phi \equiv \frac{mT_P}{MT_G} \tag{27}$$

and

$$h \equiv \frac{m(1+\alpha_P)}{2(m+M)}. \tag{28}$$

Substitution of Eqs. (25) and (26) into Eq. (20) gives

$$h(1+\phi)^{1/2}\left(1-h\frac{1+\phi}{\phi}\right) = \beta, \tag{29}$$

with

$$\beta \equiv \frac{(1-\alpha^2)\pi^{d/2}\sigma^{d-1}}{2\sqrt{2}\Gamma(d/2)Wd}. \tag{30}$$

The solution of this equation provides the expression for the temperature ratio or, more precisely for the ratio of the squares of the thermal velocities. There is a unique real solution for all allowed values of h and β. In the elastic limit, $\alpha = \alpha_P = 1$, one gets $\phi = m/M$ as required by energy equipartition. Note that all the dependence on the mass ratio and the coefficient of inelasticity for the collisions between the particles and the piston, α_P takes place through the parameter h. Equations similar to (29) have been obtained for granular systems in different contexts [34, 35, 36, 37].

The generality of Eq. (29) must be stressed. As derived, it applies not only for the steady state of the system, but for any state with gradients only in the z direction. The

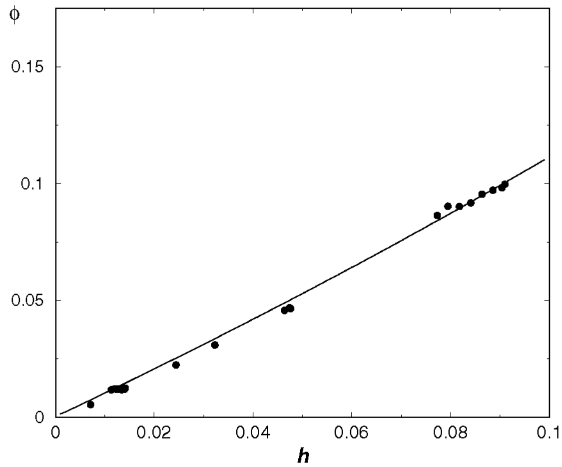

FIGURE 5. Ratio of the mean square velocities ϕ as a function of the dimensionless parameter ϕ defined in the main text. In all cases, $W = 70\sigma$ and $\alpha = 0.98$ ($\beta = 3.142 \times 10^{-4}$). The solid line is the theoretical prediction and the symbols are from MD simulations.

existence of a relationship like this is a direct consequence of the existence of normal solutions of the kinetic equations and, more precisely, of the assumption that they involve only one temperature parameter [31].

A quantitative comparison between the theoretical prediction given by Eq. (29) and the MD simulation results for the steady state is presented in Figs. 5 and 6. According with Eq. (29), for a given value of β, the value of ϕ is a function of only the parameter h. Then the comparison will be presented by considering a series of simulations in which the value of the coefficient of restitution of the gas particles α, the ratio W/σ, and, therefore, the parameter β is kept constant, while the mass ratio M/m, the restitution coefficient α_P, and, therefore, h are changed. In fig. 5 data corresponding to $W = 70\sigma$ and $\alpha = 0.98$ ($\beta = 3.142^{-4}$) are presented. A quite good agreement between theory and simulation is observed. A similar plot is shown in Fig. 6, but now for $W = 70\sigma$ and $\alpha = 0.9$ ($\beta = 1.57 \times 10^{-3}$). In this case, a clear discrepancy between theory and simulation is identified. Moreover, it increases as h increases, i.e as the mass ratio M/m decreases. Specially relevant is the discrepancy between theory and simulation when the value of α_P is changed. Upon increasing α_P and, therefore, h, the ratio ϕ is observed to decrease in a region in which Eq. (29) predicts an increasing behavior.

The curve corresponding to the theoretical prediction in Fig. 6 exhibits a very sharp minimum close to the origin. The same behavior occurs in the curve in Fig. 5, although it can not be seen on the scale of the figure. Actually, inspection of Eq. (29) shows that when h goes to zero, ϕ must tend to infinity if β is finite. An interesting behavior is obtained when h goes to zero, but $\beta' \equiv \beta/h$ remains finite. A second order phase transition occurs for $\beta' = 1$ [37]. While for $\beta' < 1$ it is $\phi = 0$ at $h = 0$ as for elastic fluids, for $\beta' > 1$, an extreme breakdown of equipartition occurs with a stationary state with $\phi \neq 0$ occurring for $h = 0$.

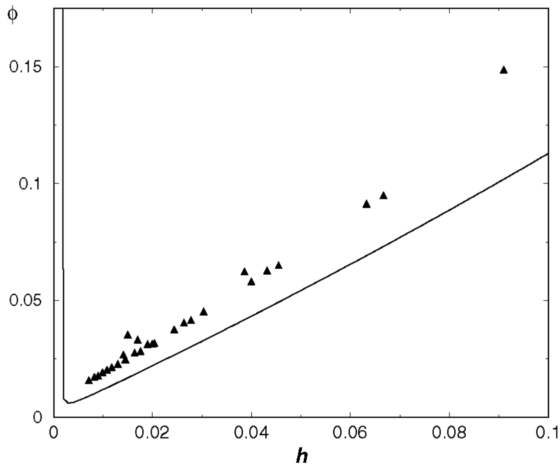

FIGURE 6. Ratio of the mean square velocities ϕ as a function of the dimensionless parameter h defined in the main text. In all cases $W = 70\sigma$ and $\alpha = 0.9$ ($\beta = 1.507 \times 10^{-3}$). The solid line is the theoretical prediction and the symbols are from MD simulations. The points aligned as an increasing function of h correspond to $\alpha_P = 1$ and different values of M/m. Those data deviating from the straight line have been obtained by varying α_P.

SUMMARY AND CONCLUSIONS

An example of the very peculiar behavior exhibited by granular systems has been presented. The steady state of a fluidized granular gas confined by a piston has been investigated by means of MD simulations. Attention has been focussed on the velocity fluctuations of the piston and of the particles in its vicinity. The results show that the temperature parameters, defined from the second moments of the velocity distributions, of the two macroscopic systems at contact may be quite different. Moreover, the relationship between them is very involved, and apparently depends on all the microscopic parameters defining the system. Although, of course, there is no conceptual paradox, since the situation considered corresponds to a far from equilibrium state, these results exemplify the difficulties when trying to define a temperature, reminiscent of the equilibrium one, for non-equilibrium systems.

A kinetic theory has been developed trying to explain the observed behavior. It is based on the Boltzmann equation for the granular gas and the Boltzmann-Lorentz equation for the motion of the piston. Assuming that the macroscopic state corresponds to "normal solutions" of those equations and that they can be generated by the Chapman-Enskog algorithm, an implicit equation for the ratio of the temperature parameter of the piston to that of the gas next to it has been derived. The solution of this equation is in good agreement with the MD simulation results for quite small inelasticity of the collisions between particles, i.e. α close to unity. Nevertheless, when the value of α decreases, the discrepancies between theory and simulations become rather strong, as it can be seen in Fig. 6.

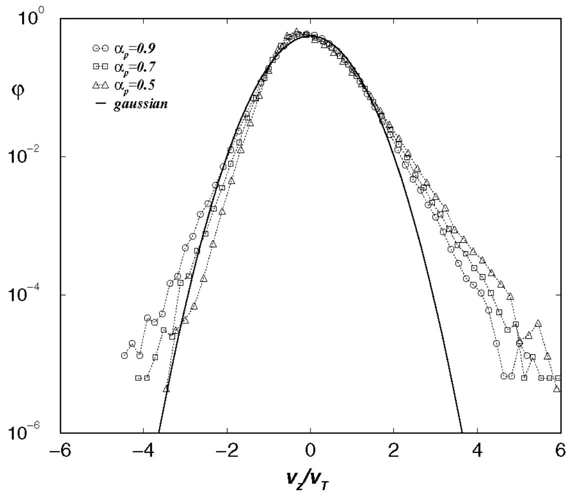

FIGURE 7. Marginal velocity distributions of the gas next to the piston in the direction perpendicular to it for several values of the coefficient of restitution α_P, as indicated. The values of the other parameters are $\alpha = 0.9, M = 49m, N = 420, W = 70\sigma$, and $v_W = 11\sqrt{g\sigma}$. The velocity is measured in the dimensionless units, $c_z \equiv v_z/v_T$.

In the theory formulated in the previous section, all the influence of the gas on the motion of the piston comes through the velocity distribution of the former just below the piston. Equation (29) was obtained by using as an approximation Gaussian velocity distributions for both the piston and the gas. As already mentioned, the simulation results show that the velocity distribution of the piston is actually Gaussian with a very high accuracy over several orders of magnitude. Then, trying to identify the origin of the failure of the theory when the inelasticity is not small, the velocity distribution of the gas next to the piston has been also measured. For $\alpha = 0.98$, the marginal velocity distribution in the direction of the gravitational field, i.e. perpendicular to the piston, turns out to be very well fitted by a Gaussian. Nevertheless, for $\alpha = 0.9$, relevant deviations from a Gaussian are observed, as shown in Fig. 7. The distribution becomes strongly asymmetric, exhibiting an exponential tail for positive velocities (towards the piston). This tail is already present well inside the region of thermal velocities, so that it affects the low moments of the distribution and, in particular the cooling rate $\zeta_P^{(0)}$.

Therefore, in order to improve the accuracy of the theoretical prediction for large inelasticity, it seems clear that a much more elaborated kinetic theory calculation is needed. The nonlinear Boltzmann kinetic equation for the gas has to be solved to get a more realistic velocity distribution for it next to the piston. Moreover, given that the MD data indicate the presence of an exponential tail for thermal velocities, an expansion in polynomials like the Sonine ones, usually employed in the context of the Chapman-Enskog expansion, may not be an appropriate strategy. This issue deserves much more attention and work.

Finally, it is worth to point out that the behavior of the piston described above opens some interesting questions, at a level both conceptual and applied. For instance, one could think of an experiment in which a molecular, elastic gas were placed on top of the piston. This gas could be confined by a higher fixed elastic wall. The question is whether the elastic gas would reach an equilibrium state with a temperature higher than the granular temperature of the gas just below the piston. The results discussed here suggest that this is the case.

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REFERENCES

1. H.M. Jaeger, S.R. Nagel, and R.P. Behringer, *Rev. Mod. Phys.* **68**, 1259–1273 (1996).
2. P.K. Haff, *J. Fluid Mech.* **134**, 401–430 (1983).
3. C.S. Campbell, *Annu. Rev. Fluid Mech.* **22**, 57–92 (1990).
4. I. Goldhirsch, *Annu. Rev. Fluid Mech.* **35**, 267–293 (2003).
5. J.W. Dufty, A. Baskaran, and J.J. Brey, *Phys. Rev. E* **77**, 031310 (2008).
6. *Granular Gases*, edited by T. Pöschel and S. Luding, LNP 564, Springer-Verlag, Berlin, 2001.
7. *Granular gas Dynamics*, edited by T. Pöschel and N. Brilliantov, LNP624, 2003.
8. A. Goldsthein and M. Shapiro, *J. Fluid Mech.* **282**, 75–114 (1995).
9. J.J. Brey, J.W. Dufty, C.S. Kim, and A. Santos, *Phys. Rev. E* **58**, 4638–4653 (1998).
10. J.J. Brey and D. Cubero, "Hydrodynamic Transport Coefficients of Granular Gases", in ref. [6].
11. V. Garzó, J.W. Dufty, and C.M. Hrenya, *Phys. Rev. E* **76**, 031303 (2007).
12. A. Baskaran, J.W. Dufty, and J.J. Brey, *Phys. Rev. E* **77** 031311 (2008).
13. L.D. Landau and E.M. Lifshitz, *Fluid Mechanics*, Pergamon, New York (1980).
14. T.P.C. van Noije, M.H. Ernst, R. Brito, and J.A.G. Orza, *Phys. Rev. Lett.* **79**, 411–414 (1997).
15. J.J. Brey, A. Domínguez, M.I. García de Soria, and P. Maynar, *Phys. Rev. Lett.* **96**, 158002 (2006).
16. I. Goldhirsch and G. Zanetti, *Phys. Rev. Lett* **70**, 1619–1622 (1993).
17. S. McNamara and W.R. Young, *Phys. Rev. E* **50**, R28–R31 (1994).
18. J.J. Brey, M.I. García de Soria, P. Maynar, and M.J. Ruiz-Montero, *Phys. Rev. E* **70**, 011302 (2004).
19. M.H. Ernst and E.G.D. Cohen, *J. Stat. Phys.* **25**, 153–180 (1981).
20. H. Wang and N. Menon, *Phys. Rev. Lett.* **100**, 158001 (2008).
21. J.J. Brey, M.J. Ruiz-Montero, and F. Moreno, *Phys. Rev. E* **63**, 061305 (2001).
22. S. McNamara and S. Luding, *Phys. Rev. E* **58**, 813–822 (1998).
23. J.J. Brey and M.J. Ruiz–Montero, unplublished.
24. J.J. Brey and M.J. Ruiz-Montero, *J. Stat. Mech.* L09002 (2008).
25. J.T. Jenkins and F. Mancini, *J. Appl. Mech.* **54**, 27–34 (1987).
26. V. Garzó and J.W. Dufty, *Phys. Rev. E* **60**, 5706–5713 (1999).
27. R.D. Wildman and D. Parker, *Phys. Rev. Lett.* **88**, 064301 (2002).
28. J.E. Galvin, S.R. Dahl, and C.M. Hrenya, *J. Fluid Mech.* **528**, 207–232 (2005).
29. J.J. Brey, M.J. Ruiz–Montero, and F. Moreno, *Phys. Rev. Lett.* **95**, 098001 (2005).
30. P. Résibois and M. de Leener, *Classical Kinetic Theory of Fluids*, Wiley-Intersicence, New York, 1977.
31. J.J. Brey, M.J. Ruiz-Montero, and F. Moreno, *Phys. Rev. E* **73**, 031301 (2006).
32. J.A. McLennan, *Introduction to Nonequilibrium Statistical Mechanics*, Prentice-Hall, Englewood Cliffs, NJ 1989.
33. J.H. Ferziger and H.G. Karper, *Mathematical Theory of Transpor Processes in Gases*, North-Holland, Amsterdam, 1972.
34. J.W. Dufty, J.J. Brey, and J. Lutsko, *Phys. Rev. E* **65**, 051303 (2002).

35. P.A. Martin and J. Piasecki, *Europhys. Lett.* **46**, 613–616 (1999).
36. J.J. Brey, J.W. Dufty, and A. Santos, *J. Stat. Phys.* **97**, 281–322 (1999).
37. A. Santos and J.W. Dufty, *Phys. Rev. Lett.* **86**, 4823–4826 (2001).