

Steady quasi-homogeneous granular gas state[☆]

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Abstract

Using Newtonian molecular dynamics we study a gas of inelastic hard disks subject to shear between two planar parallel thermal walls. The system behaves like a Couette flow and it is tuned to produce a steady state that ideally has uniform temperature, uniform density, no energy flux and a linear velocity profile for restitution coefficient in the wide range: $0.3 \leq r \leq 1$. It is shown that Navier–Stokes-like hydrodynamics fails far from the quasielastic regime. The system shows significant non-Newtonian behavior as non linear viscosity, shear thinning and normal stress differences. Our theoretical description of this state, based on generalized hydrodynamic equations derived from a moment expansion of Boltzmann’s equation, agrees reasonably well with the simulational results, and captures the non-Newtonian features of the system. We claim that our hydrodynamic equations constitute a *general formalism appropriate for describing different regimes of granular gases*.

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1. Introduction

Of all possible states of granular systems, granular gases represent a simpler not yet fully understood category [1–4]. If a granular gas is steadily “heated” by two

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parallel walls, the cooling effect of the inelastic collisions makes it reach a steady state characterized by a temperature field (*granular-temperature*) with a minimum at equal distance from these two walls [5,6]. On the other hand, a conservative gas sheared by two parallel walls with a fixed temperature T_0 , and moving in opposite directions $\pm v_0$, undergoes viscous heating and it may reach a steady state characterized by a temperature field which has a maximum equidistant from the two walls [7].

Theoretical calculations based on hydrodynamic approximations show that these two effects can cancel each other and the resulting state will have a homogeneous density and temperature as in [3] and more recently in [4,8].

This article compares the Newtonian molecular dynamics results of a two-dimensional (2D) system of inelastic hard spheres (IHS) with theoretical descriptions of a bidimensional granular gas sheared by two planar parallel walls which impose a fixed temperature T_0 at these boundaries. On carefully tuning the shearing rate—controlling v_0 —the system remains in a steady state where the two effects (inelastic cooling and viscous heating) cancel each other as much as the simulation allows. We look for the state, predicted in [3,4,8] that, at least in the bulk, has uniform temperature. This is what we will be calling a *quasi-homogeneous state* (QHS). Different authors describe the dynamics of granular gases with different hydrodynamic-like models. The most common is an extension of Navier–Stokes equations, including energy dissipation as in [2]. This is a simple procedure but, as we show here, it is inappropriate in the case of highly inelastic systems. Generalized hydrodynamics is a step forward, certainly more complex than the previous description, but nevertheless much simpler than describing the system with kinetic models. In this article we present the results obtained from our general-purpose generalized hydrodynamic equations with no ad-hoc hypothesis or adjustable parameters. These equations are able to account for the non-Newtonian behavior of the fluid observed in the simulations. A theoretical analysis of the non-Newtonian rheology of the QHS state, based on kinetic theory and moment’s method, is presented in [9]. In particular, it is shown that the effective viscosity is always different from the Newtonian viscosity obtained using the Chapman–Enskog method.

The hydrodynamic framework used in this article implies, as in previous studies, that the inelastic cooling and viscous heating can exactly cancel each other in which case all hydrodynamic fields are uniform except that the velocity profile is linear. The theoretical framework that we use is obtained from the granular-gas dynamics derived from Boltzmann’s equation using moment expansions [6] and it shows, as we will see, a quite good agreement with our own MD simulations. Our generalized hydrodynamics, described in detail in Ref. [6], is a set equations for an extended set of hydrodynamic fields (moments). Besides the usual number particle density n , velocity field \vec{v} , and temperature T , the components of the pressure tensor P_{ij} and the local energy flux \vec{Q} are considered as independent fields with their own dynamics. No constitutive relations are needed and only in simple stationary regimes with small inhomogeneities are the usual Newton and Fourier’s constitute relations obtained [10]. In two (tree) dimensions there are eight (13) independent fields. Such dynamics

was derived assuming that Knudsen's number is small; otherwise, wall effects would become dominant in the bulk of the system, spoiling the assumptions associated with moment expansions.

2. Dimensionless variables

In the following we take Knudsen's number for a system of N particles in 2D in a box $L_x \times L_y$ to be $Kn = \sqrt{\lambda/(\rho N)}$, where ρ is the area density (fraction of area occupied by the disks), and $\lambda = L_x/L_y$ is the aspect ratio. Kn is of the same order as the standard Knudsen number. Considering a system of particles of *unit mass and unit diameter* with overall number density $n_0 = N/(L_x L_y)$ and reference granular temperature T_0 , the dimensionless fields F that we use, defined in terms of the physical fields \bar{F} , are: $\bar{n} = n_0 n$, $\bar{v}_i = \sqrt{T_0} v_i$, $\bar{T} = T_0 T$, $\bar{P}_{ij} = n_0 T_0 P_{ij}$, and $\bar{Q}_i = n_0 T_0^{3/2} Q_i$. The dimensionless pressure tensor P_{ij} can be written as $P_{ij} = n T \delta_{ij} + p_{ij}$. The coordinates \bar{x}_k and time \bar{t} are related to the associated dimensionless quantities by $\bar{x}_k = L_y x_k$ and $\bar{t} = t L_y / \sqrt{T_0}$.

3. The close 8-moment solution

We assume that a stationary solution of the equations in [6] exists with a homogeneous temperature field and a disappearing y component of the velocity field. With these assumptions the mass and momentum balance equations are identities. The energy balance equation leads to

$$v'_x = - \frac{2\sqrt{2q}}{Kn\sqrt{1 - \frac{11q}{16}}} (1 - q)(3q + 2), \quad (1)$$

where $q = (1 - r)/2$ is the inelasticity coefficient, r being the normal restitution coefficient in the IHS model. The balance associated with p_{xy} yields

$$P_{yy} = \begin{cases} \frac{1}{2} \left(1 + \sqrt{1 - 4p_{xy}^2} \right), & q \leq q^* \\ \frac{1}{2} \left(1 - \sqrt{1 - 4p_{xy}^2} \right), & q > q^* \end{cases} \quad \text{where} \quad p_{xy} = \frac{\sqrt{1 - \frac{11q}{16}}}{1 + \frac{21q}{16}} \sqrt{2q}. \quad (2)$$

It is seen that p_{xy} has a maximum at the $q = q^* = 16/43 \approx 0.372093$ point at which $p_{xy} = \frac{1}{2}$. At the plastic limit $p_{xy} \approx 0.489$. Hence P_{yy} takes the sign in front of the square root according to the sign of dp_{xy}/dq .

4. A 4-fields Navier–Stokes-like solution

A granular dynamics obtained from Chapman–Enskog's method at Navier–Stokes order is much simpler than what we have been describing. It deals with three

independent fields: n , \vec{v} and T . Furthermore, the constitutive equations are Newton's law of viscous flow and Fourier's law of energy transport. One can easily find a QHS type of solution and the first important difference is that $P_{xx} = P_{yy}$ is independent of q (i.e., it falsely states that microscopically the fluid is isotropic). In the present units $P_{xx} = P_{yy} = 1$ this is in contrast with the clearly non-Newtonian behavior that the simulations show (and our higher solutions describe). Besides $P_{yy} = 1$ it gives

$$p_{xy}^{(4f)} = \sqrt{2q(1-q)} \quad \text{and} \quad v_x^{(4f)'} = -\frac{4\sqrt{2q}}{Kn} \sqrt{1-q}.$$

5. Molecular dynamics simulations

We have performed simulations of 10 000 inelastic hard disks in a box with aspect ratio $\lambda = 1$ for different values of the inelasticity coefficient q ranging from $q = 0.002$ to $q = 0.350$. There are periodic boundary conditions in the X direction while the collisions with the horizontal boundaries correspond to a contact with a heat bath at temperature $T_0 = 1$ and velocity $\pm v_0$. The area density is fixed to $\rho = 0.01$ (in which case the nonideal corrections to the equation of state are less than 2%). In the laminar (essentially one-dimensional) case under study, the interesting fields are the number density n , the granular temperature T , the longitudinal velocity v_x , two components of the pressure tensor, p_{xy} and P_{yy} , and the energy flux Q_y normal to the walls while v_y and Q_x disappear.

6. Behavior for different values of q

Since the QHS is characterized by uniform fields (taking v_x' instead of v_x) we have one value for each field for a given value of q and in this section we compare the results of the simulations with the predicted ones as a function of q . We do this from $q = 0$ to about $q = 0.35$ (restitution coefficient $r = 0.3$). Fig. 1a shows $Kn dv_x/dy$ versus q . Our theoretical solution is below the observed values. The 4-field solution fails badly for $q > 0.1$. Fig. 1b gives the values $p_{xy}(q)$. Theoretically p_{xy} should grow from zero until it takes the value $\frac{1}{2}$ to start decreasing. The values of p_{xy} from our simulations never reach $\frac{1}{2}$. In Newtonian fluids under a Couette flow, the components P_{yy} and P_{xx} of the pressure tensor are equal. In terms of our dimensionless fields this implies that $P_{yy} = 1$. From MD simulations P_{yy} differs from unity and strongly depends on q , corroborating the non-Newtonian behavior of granular gases. In Fig. 1c it is possible to verify that there is an excellent agreement between the 8-moment formalism with the simulational observation of P_{yy} . They significantly differ from unity. Finally from our data and from our theoretical expressions we have extracted the values of $\eta^* = -4p_{xy}/Kn v_x'$ which represent the dimensionless effective shear viscosity of the system. For $q = 0$ this gives $\eta^* = 1$. Fig. 2 shows the predicted and observed values which are smaller than those in the elastic case.

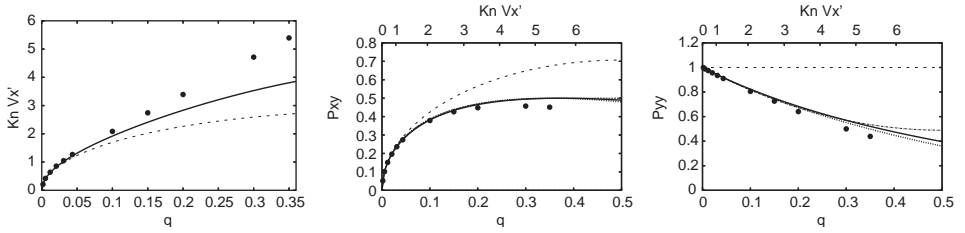


Fig. 1. In the three figures above the solid circles correspond to MD results, the solid line to the 8-moment solution and the heavy dotted line corresponds to the 4-field solution. The solution of Ref. [8] is shown by a fine line and the solution of Ref. [3] is represented by dots. The graph on the left shows $Kn dv_x/dy$ versus q . The middle graph shows the values of $p_{xy}(q)$. On the right the values of P_{yy} are shown.

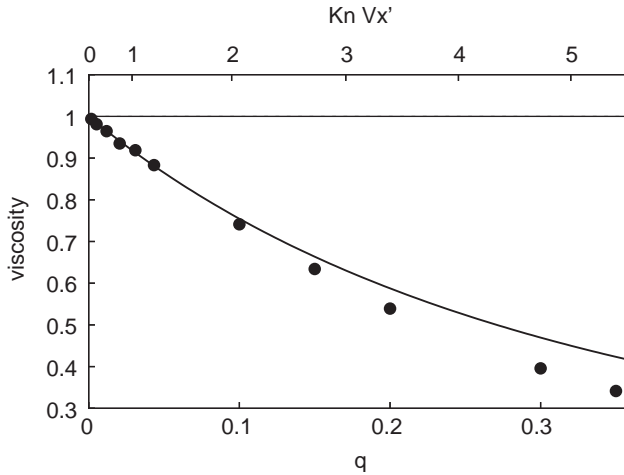


Fig. 2. The effective dimensionless shear viscosity η^* predicted here (solid line). The values obtained from MD show the same type of behavior with respect to the inelasticity coefficient q . The continuous line corresponds to the 8-moment solutions. The fine horizontal line represents the 4-field prediction.

7. Numerical comparison between solutions

In Fig. 1b we compare the values for p_{xy} given in [3,8] and the 8-moment solution. Numerically they are remarkably similar and for two of them $p_{xy}(q)$ has a maximum somewhere between $q = 0.3$ and $q = 0.4$. It is worth noting that the cited references obtain their results from solutions of the Boltzmann equation with ad hoc methods while we are using general-purpose extended hydrodynamic equations. The 4-field solution gives a $p_{xy}(q)$ which is similar to the previous solutions only for $q < 0.05$ while for larger values of q this crude approximation is much larger than the others; it is not bounded by $\frac{1}{2}$ and it has no maximum. Again the three solutions (8 moments, Ref. [3], and Ref. [8]) for P_{yy} are quite similar, and they drastically differ from the 4-field solution. The fact that P_{yy} differs so clearly from unity implies that granular

gases are non-Newtonian. This difference from the 4-fields solution, and the agreement of the generalized hydrodynamics with the MD simulations, support the idea that generalized hydrodynamics must be used to describe granular gas-dynamics. Besides, we claim that our hydrodynamic equations, based on the moment expansion method, constitute a *general formalism appropriate for describing different regimes of granular gases*. No ad hoc hypothesis or adjustable parameters are needed. Regarding the effective viscosity, while the 4-field formalism fails badly, the 8-moment solution is in good agreement with MD; see Fig. 2. The viscosity decreases as the inelasticity grows. We remark that this value of η^* cannot be predicted using the Chapman–Enskog method, which is valid only for small values of the shear rate. In fact, the viscosity computed in [11] grows with q . See a discussion on this point in [9].

8. Final comments and conclusions

We have studied a granular gas in a stationary laminar Couette state such that the viscous heating produced by a fine-tuned shearing is able to compensate the energy dissipation at collisions, giving rise to a flat temperature profile: the QHS. We were able to produce such a regime by means of molecular dynamic simulations (MD) of the IHS model with horizontal *hard and stochastic* walls and without using the Lees–Edwards or SLLOD methods, our method being closer to the experimental conditions. The analysis of the components of the pressure tensor indicates that the granular gas behaves like a non-Newtonian fluid: there is an effective non linear viscosity and the normal and transversal components of the pressure tensor are different. These properties of the fluid are expected because the shear rates are large (quantified by the dimensionless off-diagonal component of the pressure tensor).

The MD results show that the standard 4-field Navier–Stokes-like framework fails beyond the quasielastic limit and a generalized hydrodynamic theory is needed to describe granular gases. We have shown that our granular gas-dynamic equations (see Ref. [6]), once applied to the QHS, compare fairly well with the MD simulations of the granular gas for a wide range of values of the inelasticity coefficient, ranging from quasielastic states up to states not too far from the plastic limit. The agreement tends to deteriorate as the inelasticity grows but the main hydrodynamic fields are never too far from the predicted values.

The theoretical framework on which our predictions were built—and also used by other cited authors—has at its basis in the assumption that the velocity distribution function is smooth. It is known that near geometric walls this is not true. Therefore, one should expect that our predictions fail near walls and this in fact occurs.

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