Buoyancy driven convection and hysteresis in granular gases: numerical solution

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Abstract

Granular gas-dynamic equations are written down and numerically integrated to study convection. For a two-dimensional gas of inelastic hard disks in a square box and under the effect of gravity, the equations predict buoyancy driven convection triggered by the dynamically created "temperature"-gradient, in coincidence with what has been seen in molecular dynamics simulations and in real 3D experiments. Three states are observed: conductive, one-convective roll and two-convective rolls states. The numerical solution predicts a hysteresis cycle between the last two states.
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1. Introduction

In this article we study a bidimensional granular gas in a square box, subject to gravity. Three of the walls are adiabatic while the base behaves as if the system were in contact with a "heat bath". The latter plays the role of a steady energy source. The four walls are shear-free. We focus our attention in granular-gas-dynamic equations

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to prove that they predict convection driven by buoyancy effects and not by shearing effects produced by the walls of the container.

The system that we model consists of inelastic disks, all of the same size, with disk–disk collisions characterized by a constant normal restitution coefficient r. The system is in a square box, particles hitting the base bounce back preserving their tangent velocity (hence no shearing) while the normal component is sorted as if the particles were coming from a heat bath at a specified granular temperature T_0 (kinetic energy per particle). The collisions with the other three walls are mirror reflections, hence all walls are shear free. This is an unrealistic situation which has the merit of pinpointing the existence of an effect independent of external shearing. In real experiments, therefore, the combined effect of friction and inelastic collisions with the walls, plus buoyancy, must be considered when analyzing convective regimes. As a consequence of the inelastic nature of the particle–particle collisions the "temperature" will typically decrease with height. In the case of a normal fluid (i.e., with conservative collisions) in a box with isolating walls—except for a thermal base—the equilibrium is with uniform temperature regardless of the effects of gravity.

Convection in fluidized granular systems excited by a vibrating base reaching a stationary state not slaved to the movement of the base itself was apparently first suggested in Ref. [1]. We have shown—via molecular dynamics, in the case of a bidimensional system of inelastic hard disks—that if the energy injection rate comes from a shear-free stochastic base, buoyancy driven convection does appear. Buoyancy driven convection was observed in molecular dynamic simulations and it takes place as a consequence of the temperature gradient that the system dynamically creates because of the inelastic nature of the particle–particle collision rule [2]. A buoyancy driven convection of this type was then observed experimentally in a three dimensional highly fluidized granular system [3] and a theoretical calculation, based in a lattice gas Boltzmann equation, put forward to describe this type of convection, was given in Ref. [4]. See also Ref. [5].

From the theoretical point of view many proposals for granular dynamics have been submitted in the last decades [6,7]. In the case of granular gases we rely in the granular-gas-dynamic equations that we derived from Boltzmann's equation [7]. In that derivation we used moment expansions, which require a small Knudsen number. In the present case this implies that the mean free path is much smaller than the linear size of the system. The dynamic equations that we obtain are quite involved and, for the scope of the present paper, we use a simplified version of them, hoping that they grasp the basic features of the system. In the stationary case the dimensionless equations of Ref. [7] reduce, in a limit to be explained, to

$$\nabla \cdot (n\vec{v}) = 0 \ ,$$

$$n(\vec{v} \cdot \nabla)\vec{v} = -\nabla \cdot \mathbb{P} - n\,Fr\,\hat{k} \ ,$$

$$n(\vec{v} \cdot \nabla)T = -\nabla \cdot \vec{Q} - \mathbb{P} : \nabla\vec{v} - \frac{8q(1-q)}{Kn}T^{3/2}n^2 \ ,$$

where

$$\vec{Q} = -\frac{2Kn}{(1-q)(2+15q)}\, \sqrt{T}\nabla T\ ,$$

$$P_{ij} = \frac{Kn\sqrt{T}}{2(1-q)(2+3q)}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_i}{\partial x_j} - \delta_{ij}\nabla \cdot \vec{v}\right)\ ,$$

$\hat{k}$ in a unit vector pointing upward, q is the *inelasticity coefficient* $q \equiv (1-r)/2$, the Froude number is $Fr = (mgL)/T_0$, m is the mass of the disks, g is the acceleration of gravity and T_0 is the granular temperature imposed at the base. We use as Knudsen number $Kn = 1/\sqrt{N\,\rho_A}$ where N is the number of disks and ρ_A is the fraction of area occupied by the disks. This Kn is of the same order of magnitude as the ratio between the mean free path and the linear size L of the box. The general granular-dynamic equations of Ref. [7] reduce to the equations above in the limit of very small Kn. It can be seen that the mass continuity equation is the only possible one, the momentum equation is that of a Newtonian fluid with viscosity slightly different from that of an ideal gas (low density system). Something similar can be said with respect to the energy equation, except that a sink term is present. Fr, Kn plus the *inelasticity coefficient* q are the control parameters. As we have said before the aspect ratio of the box is one.

We determine—via numerical integration in a 2D grid—that the granular-hydrodynamic equations do imply that buoyancy driven convection appears when the inelasticity coefficient q is above a certain threshold. The equations are integrated in a square box having a base at fixed temperature while the other three walls are perfectly shear-free and adiabatic. The results are summarized in the following paragraphs.

We have integrated these equations for several values of the control parameters (Fr, Kn, q) and in the following we present typical results. Fixing the values $Fr = 0.55$, $Kn = 0.66$, we first get, using $q = 0$, a homogeneous solution. Then we integrate, for ever increasing values of q, taking as initial condition the last stationary solution with the previous (smaller) value of q. This is done until we reach $q \approx 0.08$, point at which we begin integrating backward, namely for decreasing values of q and again taking as initial condition the last stationary solution with the previous (larger) value of q.

In Fig. 1 we plot a simple observable, the behavior of the difference Δ between the maximum and minimum values of T at mid height, $\Delta = T_{\max} - T_{\min}$. Such difference is zero until a threshold value of q, $q_1 \approx 0.022$, where Δ starts to grow abruptly as a function of q. This change in the behavior of Δ signals the point at which convection appears for the first time. The curve then reaches a maximum and slightly beyond it, at $q_2 \approx 0.066$, Δ has a discontinuous jump to a smaller value. This transition corresponds to the passage from a one to a two-convective-rolls solution. After reaching $q \approx 0.08$ we integrate decreasing the values of q. At first we recover the same values of Δ, but the two rolls-solution remains stable below the value q_2 and a discontinuous jump to the one-roll solution occurs at $q_3 \approx 0.054$. From then on again old values of Δ are recovered. It is seen then, that there is hysteresis, namely, the discontinuous transitions take place at values of q which depend on whether q is increasing or decreasing. The statement about stability comes from the numerical
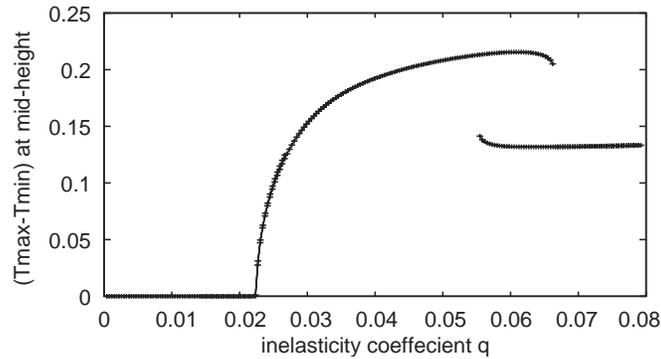
Fig. 1. Using $Kn = 0.06$, $Fr = 0.55$ and the inelasticity coefficient ranging from $q = 0$ to 0.08, the graph plots the difference Δ between the maximum and minimum values of T at mid-height. When there is no convection Δ is zero. In the zone where two stable solutions coexist, the one-roll solution has a larger Δ than the two-rolls solution. Notice the hysteresis loop.

method: if the solutions that we have found were unstable, our numerical method would have become unstable. In the case of Fig. 1 the equations in fact became unstable for larger values of q. Hysteresis when q is being varied may seem rather strange, but the point is that the numerical method shows that in a region of the parameter space there are two stable solutions and which one is obtained depends on the initial conditions.

In Fig. 2 we show the velocity $\vec{v}(x, y)$, the number density $n(x, y)$, and the temperature $T(x, y)$ for two solutions that share the same values of the control parameters: $(Fr, Kn, q) = (0.06, 0.55, 0.063)$. These two solutions were obtained keeping (Fr, Kn) fixed and approaching a value q ($q_3 \leqslant q \leqslant q_2$), from the upper and lower branches seen in Fig. 1, respectively. We have obtained solutions with both signs of the velocity field. MD simulations, on the other hand, tend to show the two rolls solution with the central part moving down and that seems to be an effect beyond our simple hydrodynamics.

2. Comments and conclusions

We have shown that our granular-gas dynamics, with shear free boundary conditions, subject to gravity and a fixed temperature at the base: (i) dynamically produces its own temperature gradient and (ii) if the inelasticity coefficient q is large enough buoyancy driven convection appears. In the bidimensional system in a square box that we have studied we obtain, numerically integrating our hydrodynamic-like equations, a purely conductive solution, a one-convective-roll solution and a two-convective-rolls solution. All of them are time-independent. Which of these solutions is reached depends on the value of the control parameters and also in the initial conditions because, as we have shown, the numerical integration method presents hysteresis. The central physical point is that there are conditions (values (Fr, Kn, q)) for which the equations have two stable solutions.
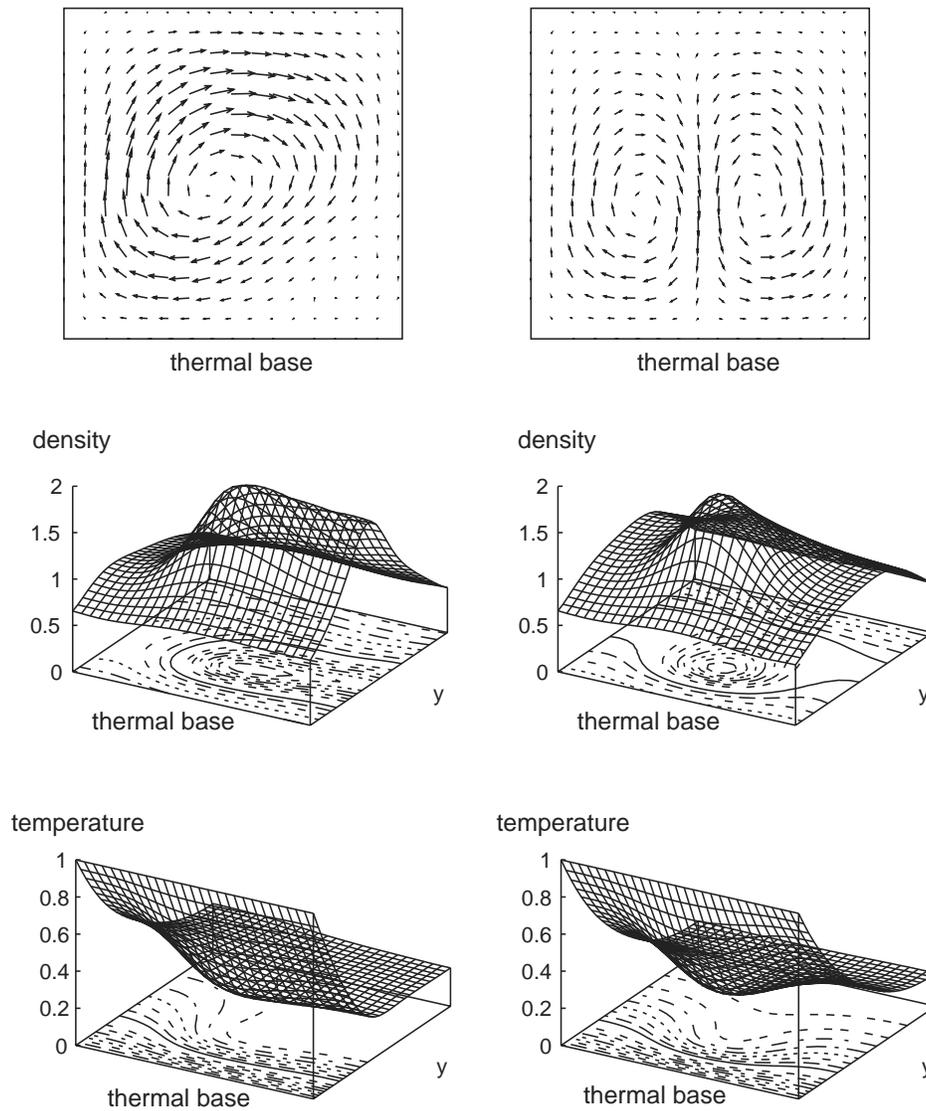
Fig. 2. Left and right figures correspond to two stable stationary solutions sharing the same values for the control parameters: $Kn = 0.06$, $Fr = 0.55$ and inelasticity coefficient $q = 0.063$. At top the velocity fields; below the surfaces representing the dimensionless number density $n(x, y)$ rescaled to satisfy $\int n \, dx \, dy = 1$; at bottom the temperature surfaces $T(x, y)$.

We finally make the distinction between the thermal boundary condition at the base and more realistic ones. Experimentally the energy source is typically a vibrating base. A granular system kept highly excited by means of a vibrating base characterized by a vibrating amplitude much smaller than the mean free path and a frequency much larger than the particle's collision rate, can behave as if it were in contact with a stochastic static wall injecting energy at a steady rate [8]. Such boundary condition is not equivalent to having the system in contact with a heat bath as defined above but they are quite similar only close to hydrostatic conditions (no convection).

Acknowledgements

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