

Thermal Convection in Fluidized Granular Systems

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(Received 9 February 2000)

Thermal convection is observed in molecular dynamic simulations of a fluidized granular system of nearly elastic hard disks moving under gravity, inside a square box. Boundaries introduce no shearing or time dependence, but the energy injection comes from a slip (shear-free) thermalizing base. The top wall is perfectly elastic and lateral boundaries are either elastic or periodic. The spontaneous temperature gradient appearing in the system due to the inelastic collisions, combined with gravity, produces a buoyancy force that, when dissipation is large enough, triggers convection.

PACS numbers: 45.70.Mg, 47.20.Bp, 47.27.Te, 81.05.Rm

In the study of granular systems, convection has attracted particular interest. Most of the experimental and simulation studies focus their attention on a granular convection mainly determined by the combined effects of a vibrating base and the roughness or inclination of the walls [1]. Also the role of voids and the effect of the internal shear bands in the system have been studied as a source of convection [2]. Some theories based on hydrodynamic continuum equations for this vibrating-base-plus-wall convection have been developed [3]. In these references the temperature gradients are considered negligible through all the medium.

However, the appearance of a convective pattern not slaved to the movement of the vibrating base has been reported in [4], suggesting the existence of a convective regime in granular systems which is not induced by the vibrating base or the walls, but it would stem from *gravity* and the dissipative nature of the granular collisions.

Although no theory is presented yet, this Letter is to clearly show the existence of this convective regime and to exhibit the mechanism that seems to be behind its origin. With this aim, our model system has no vibrating base, or any rough or inclined walls. Instead, each wall is modeled as a shear-free and time-independent boundary condition.

More precisely, we consider a granular system composed by disks interacting with a collision rule characterized by a constant normal restitution coefficient r , or equivalently, a dissipative coefficient $q \equiv (1 - r)/2$. The bottom wall gives, to each particle colliding with it, a stochastic normal component to the velocity with probability taken from a Gaussian at temperature T_0 . The tangential velocity is unchanged at the base, thus a shear-free thermal boundary condition is imposed. This boundary condition can be roughly regarded as a high frequency, low amplitude limit of a vibrating base [5]. The top wall of the system is perfectly elastic while the lateral walls are either perfectly elastic or they correspond to a periodic boundary. Particles are subjected to the acceleration of gravity g .

When energy is pumped into the granular system, through the thermal base in the present case, a temperature gradient develops spontaneously: the temperature of the

systems decreases with height. There is then an energy flux from the base upwards which is dissipated in the bulk through collisions. If the system is almost perfectly elastic it remains macroscopically static. This is the standard hydrostatic (purely conductive) regime which is observed in our molecular dynamic simulations for small values of the inelasticity coefficient q . Increasing q a transition from a conductive to a convective regime is observed in our simulations. It is argued below that this transition can be understood if we think within the frame of thermal convection, sometimes called Rayleigh-Benard convection [6].

In standard fluids the onset of thermal convection is roughly determined by the ratio between the characteristic times of the processes against convection (viscous and thermal diffusion) and favorable to convection (buoyancy). The buoyancy force is proportional to the temperature gradient, and in standard fluids it has to be externally imposed in order to observe convection. Whereas for granular systems, the temperature gradient is not externally imposed, but rather it is created by the dynamics of the system. This gradient will increase with an increasing dissipative parameter until buoyancy effects dominate, triggering convection. This means that whenever energy is injected into the system a temperature gradient develops, and unlike the case of a conservative fluid, not three but four ingredients compete inhibiting or fostering the appearance of convection: viscous and thermal diffusion, buoyancy, and *dissipation*.

This Letter reports the results about convection appearing in a 2D system—inside a box of size $L_x \times L_y$ —of N hard disks with mass $m = 1$ and diameter $\sigma = 1$, which collide inelastically with the rule

$$\vec{v}_{12}' \cdot \hat{n} = -(1 - 2q)(\vec{v}_{12} \cdot \hat{n}), \quad \vec{v}_{12}' \cdot \hat{t} = \vec{v}_{12} \cdot \hat{t}, \quad (1)$$

where $\vec{v}_{12} = \vec{c}_1 - \vec{c}_2$ is the relative velocity between the colliding particles, the primed and unprimed variables refer to the post and precollisional velocities, \hat{n} and \hat{t} are the unit vectors normal and tangential to the contact plane, with q being the dissipative coefficient as defined above. Only

translational degrees of freedom are present. The simulation results reported below come from our event-driven molecular dynamic simulations, and the careful measuring routines developed in [7].

As already mentioned, the system is maintained in a fluidized state by the injection of energy from a thermal base ($y = 0$) at temperature $T(0) = T_{\text{base}} = 1$ in energy units, while the top boundary is a perfectly elastic wall at height L . Gravity enters the problem through the Froude number, $\text{Fr} = \frac{mgL}{T_{\text{base}}}$.

We performed MD simulations for systems with a fixed number of particles, $N = 2300$, fraction of occupied area $\rho_A = 0.18$, and aspect ratio $\lambda = L_x/L = 1$, while we systematically varied the inelasticity coefficient q , in such a way that $1 \leq qN \leq 50$, and the relative gravity strength $0.1 \leq \text{Fr} \leq 2$. It was found that although the onset of convection depends slightly on the latter, the relevant parameter is qN itself. For this reason, and in order to have a clearer view of this convective phenomenon, we limit to reporting our results for $\text{Fr} = 0.1$. We want to point out that the only parameter varying from one simulation to another is q . This parameter will take values $4 \times 10^{-4} \leq q \leq 2 \times 10^{-2}$ which correspond to a restitution coefficient $0.96 \leq r \leq 0.9992$; that is, the collisions will always be quasielastic, although the macroscopic collective behavior will certainly be far from that of a standard fluid.

Convection inside a box.—Consider first the granular system inside a square box with a thermal base as described above, and perfectly elastic upper and lateral walls. In this system the boundaries introduce neither spatial nor temporal macroscopic correlations. It can be said that none of the usual conditions under which convection has been studied in granular systems are present; nevertheless, convection does appear, as observed in Fig. 1.

The hydrodynamic stationary solution for the associated conservative system ($q = 0$) is simply a constant temperature system with no heat flux and density decreasing with height. Including a small amount of energy dissipation in each collision, a conductive regime or a convective regime with one and even multiple rolls may develop into the sys-

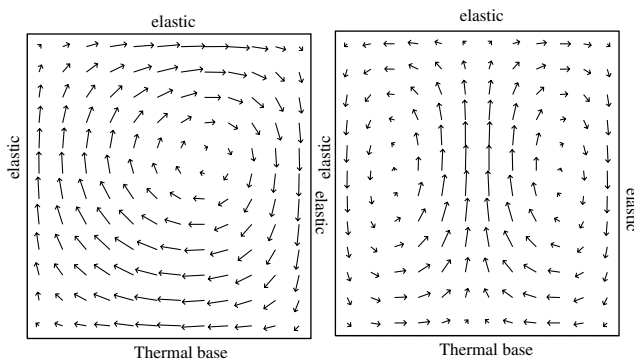


FIG. 1. Averaged velocity field for different values of qN . At the left $qN = 6$ and at the right $qN = 34$.

tem. Hence the convection we observe is due solely to gravity and the inelastic collisions between particles.

To have an insight, we have plotted (see Fig. 2) the dependence on qN of the observed granular temperature difference between the bottom ($y = 0$) and the top of the system ($y = L$), $\Delta = T(0) - T(L)$. For small values of qN this difference increases with increasing qN . This situation corresponds to the conductive regime, in which Δ can be written as an expansion on the small parameter $qN\rho_A$ [8]. This difference Δ reaches a maximum at about $qN \approx 4$, and from then on it decreases, proving that a mechanism favoring energy transport from the base upwards appears at this value. This fact is also corroborated by the amount of energy per unit time (call it heat flux) $Q(0)$, entering the system through the base, plotted in the same figure in arbitrary units. It is seen that the heat flux is steeper about the same qN for which Δ reaches its maximum: more energy per unit time is required to keep stable the temperature at the base.

From these observations we can conclude that there exists a threshold value qN from which the convection is triggered. Furthermore, this also supports the idea that convection starts when a critical value of the temperature difference between the bottom and the top of the system is reached. This convinces us that the instability is surely determined by a buoyancy force appearing with the temperature gradient, as in a standard Rayleigh convection [9].

A way to detect and quantify the transition is by measuring mass circulation in the system. This is implemented by calculating the sum of integrals of the velocity field along many concentric paths centered about the geometric center of the box: $\Phi = \sum \int \vec{v} \cdot d\vec{l}$. This observable Φ will be negligible if there is no convection and it will be distinctly nonzero (positive or negative) if there is one (anti)clockwise convective roll. Observed values of Φ are plotted in

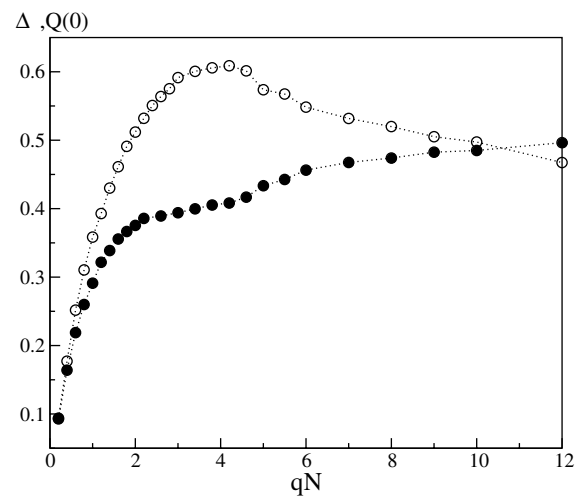


FIG. 2. Differences Δ between the bottom and top temperatures (open circles) and rescaled heat flux (solid circles) versus qN .

Fig. 3 clearly showing a supercritical transition at $qN \approx 4$ from the conductive to the convective regime with one convection roll. Because of the symmetry of the problem, rolls with both signatures are equally probable and they appear in our simulations, depending only on the initial condition.

It can also be seen that from $qN \approx 34$ up there is a coexistence of regimes with zero and nonzero circulation which corresponds to the competition of one and two convective rolls, this is, a subcritical transition from the one-roll to the two-rolls regime.

It seems to us that the appearance of the two and multi-roll regimes could be due to a change in the effective aspect ratio of the system [9]: as dissipation increases, there are regions where density rises considerably, lowering the average height occupied by the system.

Although no systematic study of higher dissipative regimes has been performed yet, we have observed that as qN continues increasing, transitions to multiroll patterns were observed but with much noise, as the system gets denser and the convective movement decreases and eventually disappears. It is in this limiting case when a nearly close packed layer of particles floating on a low density gas in contact with the thermal base is observed.

It is worth mentioning that when two rolls were observed they always appeared as shown in Fig. 1; namely, the fluid goes up in the middle of the box and comes down along the walls. This privileged signature seems to have its origin in the local increase of density that walls induce. Higher density implies more collisions and therefore more dissipation, hence lower granular temperature: the system is heavier near the walls.

Convection with horizontal periodic boundary conditions.—Any effect that the elastic lateral walls could have on the onset of convection in the previous case is discarded when periodic lateral boundary conditions are imposed on the system. The container is a periodic channel, and in this case a transition to a convective regime is found again, al-

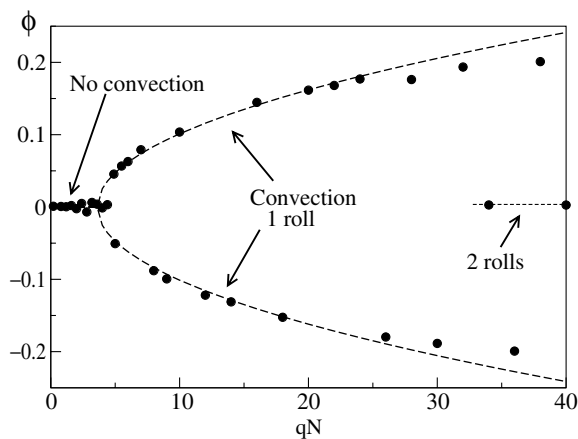


FIG. 3. Mass circulation Φ measured in simulations (points). The dashed lines correspond to the curve $\Phi = \pm 0.04\sqrt{qN - 3.8}$.

though, due to the absence of lateral boundaries, the convective rolls appearing in the system travel now along the channel. This was observed even though the simulations were carefully initialized with zero total horizontal momentum P_x , namely with zero horizontal mass flux. Since the boundary conditions do not change the horizontal component of the velocities, P_x remains zero during the evolution, as was confirmed in the simulation.

To detect this pattern, we performed time averages of the mass flux field. Because of the roll movement, this averaging time must be larger than the microscopic time and smaller than the time needed for the roll to travel a significant distance. We chose this time to be much smaller than the thermal diffusion time which, in our units, is of order $N\sqrt{\pi/T_{\text{base}}}$, but large enough to contain multiple particle-particle collisions. The observed rolls persisted for times longer than the macroscopic time, resulting in an hydrodynamic pattern.

An example of what is happening in the system is observed in Fig. 4. This figure is a plot of the averaged mass flux field at four different stages of the simulation. Because of the periodic lateral boundaries, the solution should be a two-rolls pattern (or any even number of rolls), but the aspect ratio forced on the system would imply rolls with a width about half their height, which makes them unstable. The system was most of the time observed to have one large roughly circular roll accompanied by a smaller one.

Although the movement of the rolls may be reminiscent of that spontaneously developed in the shear mode of

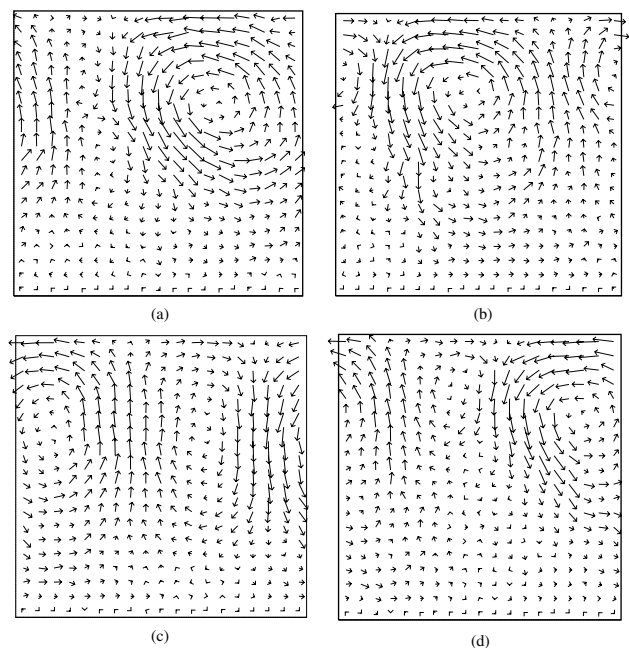


FIG. 4. Mass flux field averaged in circles of 250 collisions per particle. (a), (b), (c), and (d) correspond to cycles 100, 112, 124, and 136, respectively. A big roll can be observed moving to the left side of the system while a small roll appears varying its size.

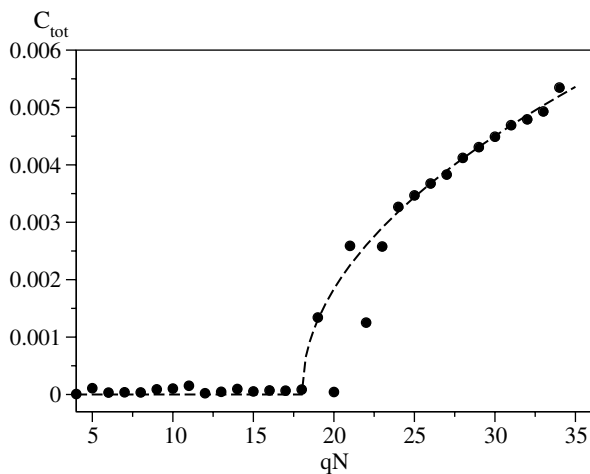


FIG. 5. Total velocity correlation C_{tot} vs qN . The transition from a conductive to a convective regime is observed at $qN \approx 18$. The data have some dispersion near the transition due to the finite size of the system. The dashed line corresponds to the curve $C_{\text{tot}} = 0.0013\sqrt{qN - 18}$.

cooling granular gases, we doubt there is a direct relation with it, since the shearing instability requires the temperature to decrease [10], while in our system the temperature remains locally constant in time.

We rather think that it is the asymmetry big/small-roll the cause of the movement of the pattern. It is well known from vortex dynamics, that a vortex near a fixed isolating wall behaves as if it were in front of a twin vortex which ensures the condition of null hydrodynamic velocity $v_y = 0$ at the top elastic wall [11]. This twin vortex would induce a movement parallel to the wall with a sense determined by the sign of the circulation of the original vortex.

In the present case, to detect the onset of convection we measured a space velocity correlation. The system is tiled with cells (i, j) and a hydrodynamic velocity correlation is defined by

$$C(i, j) = \frac{1}{8} \sum_{i', j'} \vec{v}(i, j) \cdot \vec{v}(i', j'), \quad (2)$$

where the cells (i', j') refer to the eight first neighbors of the (i, j) cell. This observable has the advantage of being insensitive to the displacements of the convective pattern. The total correlation is defined as $C_{\text{tot}} = 1/N_{\text{cells}} \times \sum_{i, j} C(i, j)$. It measures how similar, on the average, are the velocities in neighboring cells. When there is no convective pattern in the system, then the time averaged value of C_{tot} is nearly zero, while as soon as a convective current develops, C_{tot} takes distinctly positive values. Figure 5 shows the evolution of C_{tot} with qN . The transition from conductive to convective regime is clearly seen. It takes place roughly at $qN = 18$.

In conclusion, it can be stated that bidimensional granular systems exhibit convective regimes when there

is gravity and a thermal base even though no shearing is introduced through the boundary conditions. It has been shown that such convection owes its existence only to gravity and the dissipative nature of the particle-particle collisions. Because of its similarity with thermal convection in standard fluids, it has been argued that the spontaneous temperature gradient appearing due to collisions, would play the key role in this granular convection.

The authors wish to thank Professor Rodrigo Soto for helpful comments and discussions. This work has been partly financed by Fondecyt Research Grant No. 296-0021 (R. R.), Fondecyt Research Grant No. 1990148 (D. R.), and Fondecyt Research Grant No. 1970786 (P. C.).

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