Friction and convection in a vertically vibrated granular system

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The effect of friction in the thermal convection instability of granular fluids is studied by means of molecular dynamics simulations. It is found that the transitions between different convective states (zero, one, and two rolls) are primarily governed by the average energy loss per collisions and not by the friction and restitution coefficients separately, and can be roughly described in terms of a single effective restitution coefficient. The average energy loss per collisions, for a fixed value of the restitution coefficient, shows a maximum for a friction coefficient $\kappa \approx 0.3$. The presence of this maximum manifests itself as a *reentrant* behavior in the transition lines in parameter space when the value of the friction coefficient is increased beyond 0.3.

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I. INTRODUCTION

Convection is often observed in steadily vibrated granular systems and experiments tend to show that such convection is related to friction, in particular, friction between the grains and the side walls [1,2].

A few years ago it was pointed out that besides the well-known convection induced by friction with the side walls, thermal convection—similar to the buoyancy driven Rayleigh-Bénard convection—is also possible [3]. The reason for this phenomenon is that the dissipative collisions in a granular system agitated from below, inevitably produce a granular-temperature gradient which may trigger buoyancy driven convection even if there is no friction anywhere in the system. In an extreme case it was shown, via molecular dynamics with lateral periodic conditions, that convection was still observed [3]. Subsequently an experimental group observed this buoyancy driven (thermal) convection in a three-dimensional (3D) highly fluidized granular system [4]. The experiments were reproduced with 3D molecular dynamic simulations reasserting the interpretation of the experimental results [5]. A theory group obtained the same type of convection from a lattice Boltzmann gas calculation [6]. Moreover this type of convection can be obtained from the simplest granular-hydrodynamics equations [7,8] although the role of noise in a granular system where the number of particles is relatively small cannot be disregarded [9]. A quite recent and complete molecular dynamic study is in [10].

In a real system friction is inevitable and there is no doubt that in most experimental studies until now, friction with the side walls has been the dominant cause of the observed convection. It would be interesting to understand the experimental conditions under which friction and buoyancy are comparable or even the buoyancy effects are dominant. It is reasonable to think, for example, that friction with the walls becomes of little relevance far from the walls in the case of a vibrated granular system in a wide box.

In this paper, we present results concerning thermal convection in a two-dimensional system of inelastic hard disks (IHS model) subject to a vibrating base (amplitude A, angular frequency ω) in a box of dimensions $L_x \times L_y$ and with an acceleration of gravity g, in which friction is present. As it will be described in detail, friction contributes to the energy loss in collisions (as the restitution coefficients do) and therefore it affects the granular-temperature (*temperature* from now on) profile essential to have buoyancy driven convection. The collision rule, defined below, depends on the normal and tangential restitution coefficients r_n and r_t and the static and dynamic friction coefficients κ_s and κ_d. Instead of the restitution coefficients we use the inelasticity coefficients

$$q_n = \frac{1-r_n}{2}, \quad q_t = \frac{1-r_t}{2}, \tag{1}$$

which vanish for elastic collisions.

In our original work we saw that—without friction—simply varying the inelasticity coefficient q_n, the system goes from a static state to a one convective roll state and finally to a state with two convective rolls [3]. In the present study we look for the transition lines between any of these states in terms of the inelasticity and friction coefficients while $\Gamma = A\omega^2/g$ is kept fixed.

To define the collision rule we consider the collision is between two disks of mass/radius (m_1, R_1) and (m_2, R_2). A unit vector $\hat{n}$ points from the center to 2 to the center of 1, while $\hat{t}$ is tangent to the contact (its sign is immaterial). At collision the points C_1 and C_2 come in contact with relative velocity $\vec{v}$. The collision rule for two hard disks with linear momenta $\vec{p}_a$, angular velocity $\vec{\omega}_a$, and reduced mass $\mu \equiv m_1 m_2/(m_1+m_2)$ is

$$\vec{p}_1{}' = \vec{p}_1 + \vec{\Delta}, \quad \vec{\omega}'_1 = \vec{\omega}_1 - \frac{2\hat{n}\times\vec{\Delta}}{m_1 R_1},$$

$$\vec{p}_2{}' = \vec{p}_2 - \vec{\Delta}, \quad \vec{\omega}'_2 = \vec{\omega}_2 - \frac{2\hat{n}\times\vec{\Delta}}{m_2 R_2}, \tag{2}$$

where $\vec{\Delta} = \Delta_n \hat{n} + \Delta_t \hat{t}$ with Δ_n given by

$$\Delta_n = 2(1-q_n)\mu\, v_n, \tag{3}$$

while if $|v_t| < [3(1-q_n)\kappa_s]/(1-q_t)v_n$ then

$$\Delta_t = \frac{2}{3}(1-q_t)\mu\ \nu_t \text{ sticking collision rule}, \tag{4}$$

else

$$\Delta_t = \text{sgn}(\nu_t)\kappa_d\Delta_n \text{ sliding collision rule}. \tag{5}$$

The vectorial nature of the angular velocity is trivial in the sense that these are vectors perpendicular to the plane of the movement. The above collision rule was formulated by Jenkins and Zhang in a slightly different manner and it corresponds to the standard law of friction (Coulomb's law) distinguishing static and dynamic friction except that instead of taking into consideration the notion of force it is necessary to consider the instantaneous momentum exchanged [11]. It is tantamount to saying that the collision is sticking only if $|\Delta_t| < \kappa_s|\Delta_n|$ while conservation laws do the rest. If the previous inequality does not hold then $|\Delta_t| = \kappa_d|\Delta_n|$. Notice that in both cases Δ_t is proportional to the sign of $\hat{t}$ therefore $\Delta_t\hat{t}$ is independent of that sign.

Even though our system consists of disks of equal mass and radius we have preferred to write the more general rule because then it is easy to derive the dissipative collision rule with a wall. It suffices to make the limit of a disk at rest of infinite radius and mass.

Section II shows how the average energy loss per particle depends on the inelasticity and friction coefficients and how an effective inelasticity coefficient can be defined. In Sec. III two order parameters are used to characterize the different convective regimes and, with their help, our different simulational data are described. Transition lines are found in the κ-q plane to separate regions where there is no convection, one convective roll, two convective rolls, or even collapse. A summary and conclusions are found in Sec. IV.

II. AVERAGE ENERGY LOSS PER COLLISION

As it has been said, thermal convection takes place because the energy being pumped through the vibrating base keeps the grains near the base well agitated while they are increasingly slower (cooler) at higher altitudes. This implies a temperature gradient dynamically created by the loss of energy in every collision.

How sensitive is the convection process to the way the energy is lost? For example, the inelasticity coefficients can be set to zero so that all the energy loss is due to friction or, in the other extreme, the friction coefficients may be set to zero, tuning the inelasticity coefficients to have the same average energy loss per collision as before. Would convection be the same or how different would it be? Furthermore, can the combined effect of friction and inelasticity be put together into a single effective inelasticity coefficient?

One can check that in every collision between two disks of equal mass m the instantaneous energy change dE in a sticking collision is

$$dE = -q_n(1-q_n)m\nu_n^2 - q_t(1-q_t)m\nu_t^2, \tag{6}$$

while if there is sliding then

$$dE = -(1-q_n)[(q_n - 3(1-q_n)\kappa_d^2)m\nu_n^2 + \kappa_d m|\nu_t|\nu_n]. \tag{7}$$

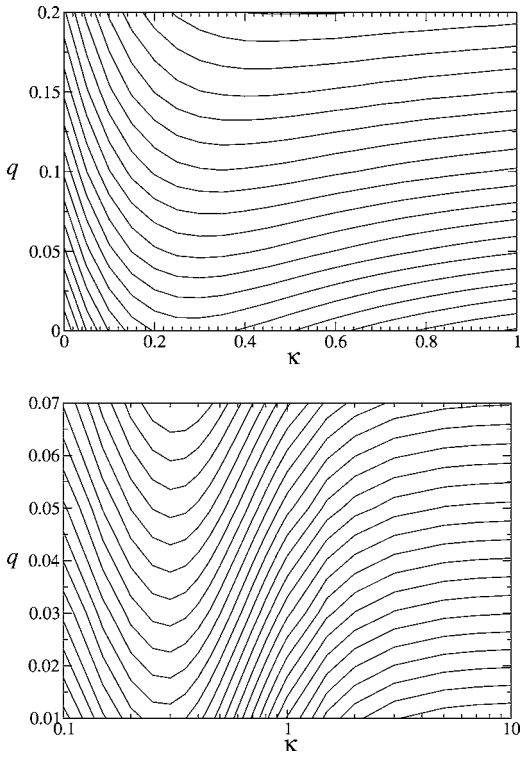

FIG. 1. Lines of equal Monte Carlo mean energy loss per collision $\langle dE\rangle$ in the κ-q plane. Lower lines represent less energy loss. Top: whole range $0 \leqslant q \leqslant 0.2$. Bottom: Detail for small q values using logarithmic scale in the κ axis. It can be seen that in this range of q varying κ from zero upward with q fixed, the absolute value of the Monte Carlo mean energy loss increases until $\kappa \approx 0.3$ and then $|\langle dE\rangle|$ decreases again.

As a first step, before tackling the molecular dynamic study, we have made a simplified evaluation of the mean energy loss per collision $\langle dE\rangle$ evaluating the phase-space statistical mechanics integral which defines such average. With this aim we have made the rather crude assumption that locally particles have a Maxwellian distribution and, we have used the Monte Carlo integration technique [12] to evaluate the average $\langle dE\rangle$ using the collision rule of Sec. I.

Since the collision rule does not depend on the energy scale but only on dimensionless parameters, the temperature for the Maxwellian distribution has been set equal to unity without losing generality. The results, in the form of the iso-$\langle dE\rangle$ curves are shown in the κ-q plane in Fig. 1. For simplicity we have taken equal inelasticity coefficients $q \equiv q_n = q_t$ and equal friction coefficients $\kappa \equiv \kappa_d = \kappa_s$. In the figure it is particularly clear that the mean energy loss $|\langle dE\rangle|$ has a maximum when $\kappa \approx 0.3$.

A rough argument to understand the existence of this maximum follows. The condition determining whether a collision is sliding or sticking says that for low values of κ most collisions are sliding and as the friction coefficient is small, the energy loss is mainly due to the normal inelasticity coefficient. For large values of κ, collisions are mainly sticking and again the energy loss does not depend on κ but only on the inelasticity coefficients. Therefore, the role of κ in the energy loss manifests itself only for intermediate values of κ,

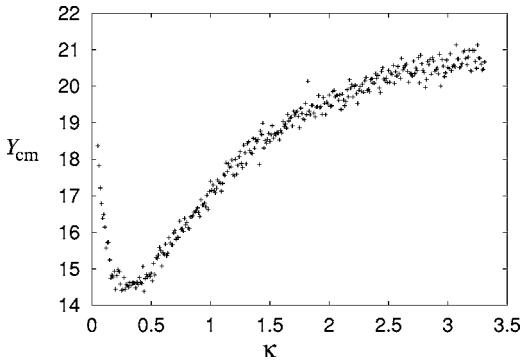

FIG. 2. The average height Y_{cm} of the center of mass of a system (in units of particle's diameters) of inelastic disks as a function of the friction coefficient κ. The minimum is at about $\kappa \approx 0.3$

and the Monte Carlo mean value shows that it is largest at $\kappa \approx 0.3$. Furthermore, the absolute value of the *instantaneous* energy loss in a sliding collision, given in Eq. (7), regarded as a function of κ_d, has a maximum at $\kappa_d^{\max} = |\nu_t|/[6\nu_n(1-q_n)]$ which suggests that $\kappa_d^{\max}$ moves to the right for more inelastic collisions (larger q) which is what is seen in Fig. 1. It also gives the correct order of magnitude of the position of the maximum.

Note that the particular value for the largest energy loss per collision was obtained by Monte Carlo averaging using $q_n = q_t$ and $\kappa_d = \kappa_s$. We have checked that changing the relative values of the inelasticity coefficients does not much affect the position of the maximum, always being close to 0.3, which is consistent with the previous paragraph.

To further check that $\kappa \approx 0.3$ corresponds to the largest energy loss for nearly elastic collisions we performed a series of molecular dynamic simulations to study the average height of the center of mass of a granular system excited from the base, as a function of κ keeping the inelasticity coefficients small and fixed. Figure 2 shows the average height of the center of mass of a system with $N=500$ disks of unit diameter and mass, $g=0.002$ and stochastically excited from the base with a thermal base characterized by $T_0=1$. The width of the box is $L_x=25$ and there is no ceiling. This is a narrow box to avoid convection. The inelasticity coefficients are $q_n=q_t=0.025$ and the particle-particle and particle-wall friction coefficients κ are the same. If the system were in close packing there would be slightly more than 20 layers of grains and the height of the center of mass would be about $5\sqrt{3} \approx 8.7$. Figure 2 shows that the system becomes more compactified at $\kappa \approx 0.3$, still much looser than close packing. This is consistent with a maximum energy loss $|\langle dE \rangle|$ at this value.

In the case when there is no friction all the energy loss comes from the value of q_n and assuming a Maxwellian distribution the mean energy loss per collision is

$$\langle dE \rangle = -4q_n(1-q_n)T_0 \tag{8}$$

then, for the general case including friction, given the value of $\langle dE \rangle$ one can define an *effective normal inelasticity coefficient* by

$$q_{\text{eff}} \equiv \frac{1}{2}\left(1 - \sqrt{1 + \frac{\langle dE \rangle}{T_0}}\right), \tag{9}$$

where $T_0=1$ is the temperature used in the Maxwellian.

The results shown in Fig. 1 indicate that q_{eff} is monotonic in q but the dependence on κ has a maximum close to $\kappa \approx 0.3$.

In Ref. [3] thermal convection was studied in the absence of friction. The only dissipative coefficient was q_n and the threshold values of q_n to transit from zero to one roll and from one to two rolls were found. Since the convective instability is mainly triggered by energy dissipation, it can be expected that, in the presence of friction, the location of the, say 0 to 1 roll transitions, will take place—in the (κ, q) plane—when $\langle dE \rangle$ takes (roughly) the same characteristic value. Thresholds, of course, depend on Γ.

In the following section we analyze the molecular dynamic behavior of a bidimensional system of hard disks obeying the collision rule described in the Introduction.

III. SIMULATIONS

We perform molecular dynamic (MD) simulations of inelastic hard disks interacting with the collision rule described by Eqs. (2)–(5). The simulational setup consists of $N=1000$ disks of unit mass and diameter $\sigma=1$ in a rectangular box of width $L_x=60\sigma$ and height $L_y=150\sigma$. The grains are fluidized by the movement of the base, which is subject to a vertical oscillation with amplitude $A=0.1\sigma$ and frequency $f=\omega/2\pi$, with $\omega=10$ [13]. The movement corresponds to a piecewise constant acceleration that mimics a sinusoidal oscillation. We choose gravity big enough so that collisions with the upper wall are rare. Again, for simplicity, we take $q \equiv q_n = q_t$ and $\kappa \equiv \kappa_d = \kappa_s$; and we use the same inelasticity and friction coefficients for grain-grain and grain-wall collisions including the oscillating base. Going beyond that would be a tremendous task far beyond the scope of the present article.

A. Order parameters

To identify the convection states we define two order parameters Ψ_1 and Ψ_2

$$\Psi_1 = \frac{1}{N}\sum_{i=1}^{N} \nu_{yi} \sin(2\pi x_i/L_x), \tag{10}$$

$$\Psi_2 = -\frac{1}{N}\sum_{i=1}^{N} \nu_{yi} \cos(2\pi x_i/L_x), \tag{11}$$

where (x_i, ν_{yi}) are the x-coordinate and y-velocity components for particle i. Both order parameters vanish when the granular fluid is static (no convection has developed). Having one convective roll, Ψ_1 is distinctly nonzero and depending on the position of the locus of the roll, Ψ_2 can be negative, zero, or positive. Ψ_1 is positive (negative) if the roll circulates (counter) clockwise. When two symmetric rolls are present, Ψ_1 vanishes and Ψ_2 is nonzero, being positive if the granular fluid goes upward in the middle of the box and

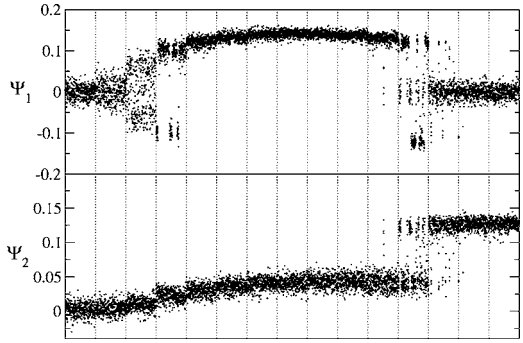

FIG. 3. Example of the evolution of the order parameters Ψ_1 and Ψ_2 when changing κ for fixed $g=0.015\,625$ and $q=0.0$. Within each vertical bin, the value of κ is kept fixed and the points correspond to the instantaneous values of the order parameters, taken every 100 oscillations of the base. Between vertical bins, the value of κ is increased by 0.005, starting from 0.005 and in the last bin $\kappa=0.075$.

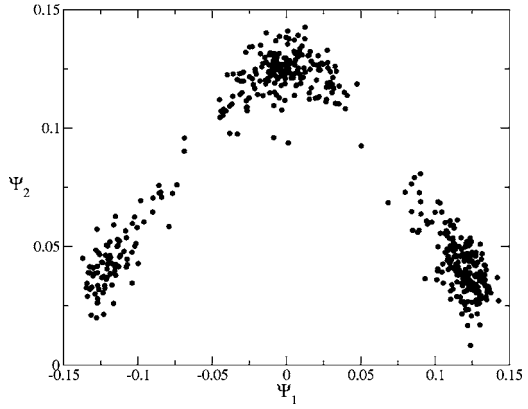

FIG. 4. Plot of the order parameter values in the plane (Ψ_1,Ψ_2) for a condition with coexistence between 1 and 2 rolls: $q=0.0$, $\kappa=0.0605$, and $g=0.015\,62$. The top cluster corresponds to two rolls, and the right and left clusters to one roll, circulating clock or counterclockwise, respectively.

descends by the lateral walls; otherwise it is negative.

The system is left to evolve for 10^5 oscillations of the base before changing any control parameter. The order parameters are evaluated regularly every 100 oscillations of the base. This gives a total of 1000 measurements per value of the control parameter. The first 500 measurements are discarded (possible initial transient) and the next 500 measurements are considered to characterize the state of convection. After the 10^5 periods, the control parameter κ is slightly increased starting the new simulation from the final configuration of the previous case. A typical plot of the time evolution of the order parameters, while increasing the friction coefficient, is shown in Fig. 3. At first there is a continuous transition from a conductive (static) regime to a one-roll convective state, showing jumps from clockwise to counterclockwise rolls. Higher up in κ there is a discontinuous transition from one to two rolls ($\Psi_1=0$) and back. This transition exhibits also a region of coexistence between one and two rolls before the state stabilizes in a two-roll state. Jumps between the coexisting states (clock/counterclockwise rolls and one/two rolls) are observed because there is a finite number of particles.

To precisely identify the average order parameter values, in the case of the coexistence of two states we plot, for each value of the control parameter, the last measured 500 points in the plane (Ψ_1,Ψ_2) as in Fig. 4. A *K*-means cluster classification technique is used to determine the characteristic mean values that correspond to each state [14]. Figure 4 shows a typical three-cluster graph in the case of coexistence of a clockwise and counterclockwise one-roll and two-roll states.

B. Thresholds in the κ-q plane

Two series of molecular dynamic simulations were performed, with $g=0.002\,025$ ($\Gamma\approx 4938$) and with $g=0.015\,625$ ($\Gamma=640$) [13], varying κ and q in order to identify the convective transitions already described. In both series we observed regions in the κ-q plane without convective rolls, with one and two rolls or *collapsed* states (states with a big upper compact layer on top of a gas-like region). The states with two rolls always have $\Psi_2>0$, indicating that the granular fluid goes up in the middle of the box and descends by the walls. Figure 5 shows the transition lines between states with zero, one, and two convective rolls. Both graphs are in the $\ln(\kappa)$-q plane. The transition lines follow a tendency similar to the iso-$\langle dE\rangle$ curves. In particular the value $\kappa\approx 0.3$ again appears as the value where the energy loss is the largest. Also, the fact that the energy loss per collision has a maximum for $\kappa\approx 0.3$ produces *reentrant* transitions, when increasing the value of κ. These results confirm that in the present case convection is triggered by the energy dissipation which induces buoyancy. The mechanisms which produce energy loss in every collision do not seem to be relevant.

The second series of simulations—with larger gravity—has a denser system, hence there is a larger collision rate and therefore more energy is dissipated per unit time. Hence the transition lines are seen at lower values for the inelasticity coefficient. In this case (larger gravity), convection transitions (and collapse) can be observed even at $q=0$.

Hysteresis is observed in the transition between the states with one and two rolls, whereas no hysteresis is detected in the other transitions. The coexisting region is relatively small in parameter space, but nevertheless it can be easily characterized as observed in Figs. 3 and 4.

Next we study to what extent the transition lines can be characterized by a single value of $\langle dE\rangle$. Namely, we put to test the hypothesis that it is the mean energy loss per collision and not particular values of q and κ which describe the type of convective state of the system. For every point in the κ-q space—corresponding to each transition line—we have evaluated $\langle dE\rangle$. The average of these values, with the corresponding standard deviations, are seen in Table I. The table shows that for every transition line (considering the low and high κ branches) the values of the mean energy loss per collision are similar and clearly different from those of the other lines, except, of course, between the very close lines

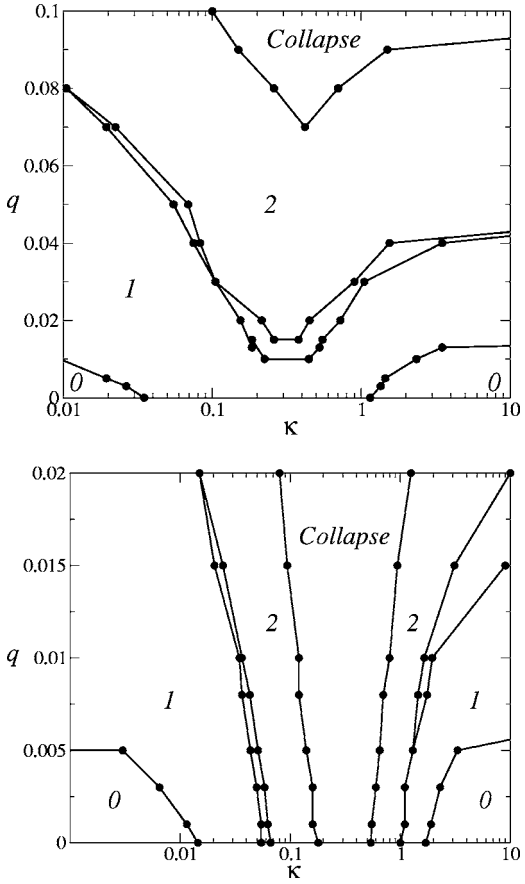

FIG. 5. Convective states displayed in the $\ln\kappa$-q parameter space. Gravity is $g=0.002\,025$ on the top graph and $g=0.015\,625$ on the bottom graph. The labels "0," "1," and "2" represent states with 0, 1, and 2 rolls, respectively, while the label "Collapse" represents the collapsed state described in the text. Dots are the values obtained in the simulations and the lines are drawn to help read the graph. The transition from the states with one and two rolls shows hysteresis and therefore, there are two associated transition lines, indicating the beginning and the end of the coexisting region.

associated to hysteresis. The conclusion is that the buoyancy driven convection states reported here are dominantly determined by $\langle dE\rangle$ and hence can be described by an effective dissipation coefficient q_{eff} as in Eq. (9). Hence, at least approximately, we can state that convection does not depend on the dissipation and friction coefficients separately. This effective description is not completely accurate and the main source of discrepancy comes from the fact that the velocity distribution is not Maxwellian [15] and that the translational and rotational temperatures are typically different [16]. A more detailed study shows that the transport coefficients, that are involved in the convection thresholds, depend on the friction and dissipation coefficient separately [17]. A possible manifestation of these phenomena is the fact that although the values $\langle dE\rangle(\kappa,q)$ within each transition line are similar, there is a weak dependence on q: to larger values of q correspond slightly smaller values of $\langle dE\rangle$.

Finally, we stress that we are not stating that the quantitative convective currents are independent of the particle-wall friction coefficient, but that this phenomenon is driven by bouyancy and not by the stresses at the walls; thermal convection exists even without friction. We expect that changing the particle-wall friction but keeping q_{eff} constant will somehow quantitatively change the convective phenomenon but Fig. 5 shows that the thresholds follow the shapes seen in Fig. 1.

IV. SUMMARY AND CONCLUSIONS

Using MD simulations of granular fluids with particle-particle and particle-wall collisions, characterized by inelasticity and friction, we have shown that buoyancy driven convection develops even when inelasticity vanishes. For different values of the inelasticity coefficient q and the friction coefficient κ it is observed that there are transition lines (in the κ-q plane) from zero to one convective roll, from one to two rolls (with hysteresis), and from two rolls to *collapse*.

The study of the statistical mechanics mean energy loss per collision $\langle dE\rangle$ assuming a Maxwellian velocity distribution leads to the conjecture that there are reentrant transitions in the sense that increasing the friction coefficient κ beyond the value 0.3 there are successive transitions similar to those observed below $\kappa\approx 0.3$ but in reverse order. The conjecture is confirmed by our MD simulations.

The idea that it is possible to give a qualitatively correct though approximate description of the behavior of the system using a unique dissipative coefficient q_{eff} to encompass

TABLE I. Monte Carlo mean energy loss per collision $\langle dE\rangle$ averaged over all points of a transition line and the corresponding value of the effective inelasticity coefficient q_{eff}. The transition from one to two rolls is separated in (a) the beginning of the coexisting region and (b) the end of the coexisting region.

g	Transition	$\langle dE\rangle$	q_{eff}
0.002025	0-1	-0.090 ± 0.017	0.023 ± 0.004
	1-2(a)	-0.351 ± 0.042	0.097 ± 0.013
	1-2(b)	-0.377 ± 0.046	0.105 ± 0.014
	2-collapse	-0.614 ± 0.036	0.190 ± 0.014
0.015625	0-1	-0.047 ± 0.009	0.012 ± 0.002
	1-2(a)	-0.137 ± 0.022	0.035 ± 0.006
	1-2(b)	-0.147 ± 0.025	0.038 ± 0.007
	2-collapse	-0.290 ± 0.037	0.079 ± 0.011

the combined effect of the inelasticity and friction coefficients is confirmed both, by the qualitative similarity between the curves in Figs. 1 and 5, and most importantly, by the fact that the transitions are quite well characterized by the value of the mean energy loss $\langle dE \rangle$ as seen in Table I. Hence, defining an effective inelasticity coefficient q_{eff} is approximately correct.

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