Understanding the instability of a vibrated granular monolayer

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We investigate the dynamics of an ensemble of inelastic hard spheres confined between two horizontal plates separated a distance smaller than twice the diameter of the particles, in such a way that the system is quasi-two-dimensional. The bottom wall is vibrating and, therefore, it injects energy into the system in the vertical direction and a stationary state is reached. It is found that, if the size of the plates is small enough, the stationary state is homogeneous. Otherwise, a cluster of particles is developed. The instability is understood by using some effective hydrodynamic equations in the horizontal plane. Moreover, the theoretical prediction for the size of the system above which it is unstable agrees very well with Molecular Dynamics simulation results without any fitting parameter.

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A granular system is an ensemble of macroscopic particles, named grains, that interact via inelastic collisions. When two grains collide, due to its macroscopic character, part of the kinetic energy associated to the center of mass of the particles is dissipated exciting other degrees of freedom. Hence, besides the fact that granular matter is ubiquitous in Nature, these systems are very interesting from a theoretical point of view because they are intrinsically out of equilibrium [1].

Experimentally, it is relatively easy to generate stationary states by just vibrating the walls of the container of the system. In these states, the energy injected in the system is compensated by the energy dissipated at collisions. The price to be paid is that the steady state is highly inhomogeneous, as can be understood from the generalized Navier-Stokes equations describing the dynamics of the system [2]. An exception to this is a granular system placed in a vertically vibrated quasi-two-dimensional (Q2D) shallow box. In this case, the stationary state can be homogeneous when projected in the horizontal plane and, when observed from above, the system behaves as a two-dimensional fluid. Actually, in the last years, many experiments have been performed under these conditions [3, 4]. Experiments can be carried out with or without a top lid, being gravity in the last case the responsible of the Q2D confinement.

Typically, the grains are confined between two plates separated a distance $H$ smaller than twice the diameter of the particles, so that they can not jump on to each other and the system can be considered to be Q2D. The bottom wall is vibrated sinusoidally with frequency $w$ and amplitude $A$ that is always much smaller than the height of the system, i.e. $A << H$. Most of the experiments are performed with smooth plates although in some cases a rough one is used [4]. The particles gain energy in the vertical direction through collisions with the bottom wall and it is transferred to the horizontal direction via collisions between particles, where energy is also dissipated. Experiments show that, for a wide range of the parameters, the system reaches a homogeneous stationary state. On the other hand, it is also observed that the system becomes unstable by increasing the density and/or decreasing the dimensionless parameter $\Gamma = \frac{4w^2}{g}$, $g$ being the gravitational acceleration [3, 5, 6]. In particular, there is a regime in which an aggregate surrounded by a hotter gas is formed. In the last years, there have been many efforts to understand this phenomenology. For example, it is known that, in the context of hydrodynamics, the instability is triggered by a negative compressibility in the associated horizontal equation of state [7, 10] and some of the phases have been characterized [6, 7]. Nevertheless, there are still many points that are not clear. In particular, what are the essential ingredients to have this kind of instability?, why is the compressibility negative?, can the equation of state in the horizontal plane be derived from a microscopic point of view? In any case, what is the mechanism that stabilizes/distabilizes the system? In order to tackle these questions some two dimensional (D) models have been considered. As the system is Q2D, it is expected that the actual 3D dynamics could be substituted by an effective 2D dynamics in which energy is injected by some kind of mechanism as, for example in the 3D stochastic thermostat [11] or in the so-called $\Delta$ model [12]. Nevertheless, both models have been extensively studied finding that the homogeneous stationary state that is reached in the long time limit is always stable [13, 14]. Very recently, a new 2D model has been formulated in which the homogeneous stationary state is unstable [15], but the proposed microscopic dynamic is defined in terms of some parameters that, in principle, must be fitted.

The objective in this paper is to introduce the simplest model that captures the phenomenology of the experiments and that let us understand the origin of the instability. To properly describe the energy transfer from the vertical to the horizontal direction, we consider a simple 3D model: an ensemble of $N$ inelastic hard spheres of mass $m$ and diameter $\sigma$, confined between two flat
planes located at \( z = 0 \) and \( z = H \). It will be assumed that \( H < 2\sigma \) so that the system is Q2D (see Fig. 1). The plates are square shaped of area \( L \times L \) with \( L \gg H \) and periodic boundary conditions are used in the horizontal direction. The collisions between the particles are inelastic, characterized by a constant (independent of the relative velocity) coefficient of normal restitution, \( \alpha \) \( (0 \leq \alpha \leq 1) \), being the collisions elastic for \( \alpha = 1 \). The collisions with the top wall are elastic, so that the horizontal component of the velocity does not change and \( v_z \rightarrow -v_z \). The bottom wall will be modeled by a sawtooth wall of velocity \( v_p \). This kind of wall mimics the dynamics of a wall that moves sinusoidally in the limiting case \( A \rightarrow 0, w \rightarrow \infty \) with \( Aw = v_p \). When a particle collides with the bottom wall, its horizontal velocity remains unchanged while \( v_z \rightarrow 2v_p - v_z \). This kind of collision always injects energy into the system. The total horizontal momentum of the system is, then, a constant of motion.

We have performed Molecular Dynamics (MD) simulations of the model finding that it fulfills the desired conditions: for a wide class of values of the parameters the system reaches a homogeneous stationary state and, when increasing the density, a dense cluster surrounded by a gas is developed. In Fig. 2 a snapshot of a configuration of a MD simulation where the cluster is formed is shown (the system is seen from above). The parameters of the simulations are \( N = 2000, \alpha = 0.9, H = 1.5\sigma, L = 115\sigma \) and \( v_p = 0.01\left(\frac{2T(0)}{m}\right)^{1/2} \), where \( T(0) \) is the initial horizontal temperature.

The objective now is to understand, first, the homogeneous two-dimensional phase and, second, the origin of the instability. To study the homogeneous phase, we will admit, in the same spirit that in Ref. [10], the existence of a closed description in terms of the 2D density, \( n \), the horizontal temperature, \( T \), and vertical temperature, \( T_z \). The idea is that, as energy is injected in the vertical direction and transfer to the horizontal direction through collisions, this is the minimal number of variables to understand the dynamics of the homogeneous system. Total momentum in the plane does not play any role in this context as it is a constant of the motion. In the low-density limit, assuming that the system is very thin, i.e. \( \epsilon \equiv \frac{H-\sigma}{\sigma} \ll 1 \), and that the collisions between particles are nearly elastic, \( 1 - \alpha \ll 1 \), the evolution equations are

\[
\frac{dT}{dt} = 2\sqrt{\frac{\pi}{m}}n\sigma T^{\frac{1}{2}}\left[-(1-\alpha)T + \frac{\epsilon^2}{3}(T_z - T)\right], \tag{1}
\]

\[
\frac{dT_z}{dt} = -\frac{4}{3}\sqrt{\frac{\pi}{m}}\epsilon^2 n\sigma T^{\frac{1}{2}}(T_z - T) + \frac{2v_p^2}{\sigma^2}T_z. \tag{2}
\]

Let us discuss briefly each term in the equations. The first term in the right hand side of Eq. (1) describes the energy loss due to inelastic collisions between particles and the 2D expression has been taken [1]. The second term is the kinetic energy transfer from the vertical to the horizontal direction that is proportional to the difference of temperatures times the thermal horizontal velocity. We have taken the elastic limit calculated in [17] from kinetic theory tools. This term also appears in Eq. (2) but with a different sign and multiplied by \( 2 \) due to the difference in the definition of temperature in terms of energy. Finally, the second term in the right hand side of (2) describes the energy injection due to the vibrating wall. In this case, the term can be evaluated exactly as it is proportional to \( v_p \) times the pressure of the granular gas just above the vibrating wall in the direction perpendicular to it [18]. In fact, these equations can be derived from a kinetic equation for the monolayer by an expansion in \( \epsilon \) and assuming that the velocity distribution function is a Gaussian with two temperatures [19]. The only difference is that the energy transfer terms have a non-trivial dependence on \( \alpha \) neglected in the present case.

Eqs. (1) and (2) admit only one stationary solution, \( T_s \) and \( T_{z,s} \), that can be easily calculated as functions of the inelasticity, density and dimensionless height, \( \epsilon \). From Eq. (1) the quotient of the stationary temperatures, \( \gamma \equiv \frac{T_{z,s}}{T_s} \), is

\[
\gamma = 1 + \frac{3(1-\alpha)}{\epsilon^2}. \tag{3}
\]
Remarkably, it is proportional to \( n^{-2} \), so that the pressure in the stationary state goes as \( n^{-1} \), and the compressibility of the non-equilibrium steady state is negative. Note that this dependence is a direct consequence of the particular way in which energy is injected and transferred in the monolayer.

In order to see that Eqs. (1) and (2) describe correctly the dynamics of the system, we have performed MD simulations measuring the time evolution of the horizontal and vertical temperatures. We have considered different densities (below \( n\sigma^2 = 0.03 \)), heights (below \( \epsilon = 0.5 \)) and coefficients of normal restitution (above \( \alpha = 0.9 \)), checking that the system stayed always homogeneous. Of course, those cases in which the instability showed up were discarded. For all the considered initial conditions (that was taken to be a Gaussian with two temperatures), the numerical solution of the equations agrees very well with the simulation results for all times and, in particular, with their stationary values given by Eqs. (3) and (4). This is remarkable since there are not any adjustable parameter.

A stability analysis of Eqs. (1) and (2) shows that the stationary solution is linearly stable. In fact, the matrix associated to the dynamics of the stationary solution is linearly stable. In fact, the two constants \( n_s \) and \( T_s \) must be related by Eq. (4) that has to be equivalent to \( G(n_s, T_s(n_s)) = 0 \). The objective now is to study if this state is linearly stable. To do that, it is convenient to introduce the dimensionless deviations of the fields around the homogeneous solution \( \rho \equiv \frac{n - n_s}{n_s} \), \( \mathbf{w} \equiv \sqrt{\frac{m}{2T_s}} \mathbf{u} \) and \( \theta \equiv \frac{T - T_s}{T_s} \), as functions of the dimensionless time scale, \( s \), and dimensionless space variable \( l \equiv n_s \sigma \mathbf{r} \). Let us also introduce the Fourier components of these functions through \( y_k \equiv \int dl e^{-ikl} y(l) \) and let us decompose \( \mathbf{w}_k \) into its parallel, \( \mathbf{w}_{k\parallel} \equiv \mathbf{w}_k \cdot \hat{\mathbf{k}} \), and transversal \( \mathbf{w}_{k\perp} \equiv \mathbf{w}_k \times \hat{\mathbf{k}} \) components (\( \hat{\mathbf{k}} \) is a unit vector perpendicular to \( \mathbf{k} \)). The evolution equation for the transversal component is \( \frac{\partial}{\partial s} \mathbf{w}_{k\perp} = -\mathbf{q}_{k\perp} \), that is decoupled from the rest of Fourier components, that verify

\[
\frac{\partial}{\partial s} \begin{pmatrix} \rho_k \\ w_{k\parallel} \\ \theta_k \end{pmatrix} = \mathbf{L} \begin{pmatrix} \rho_k \\ w_{k\parallel} \\ \theta_k \end{pmatrix},
\]

where we have introduced the dimensionless time \( ds = n\sigma \sqrt{\frac{2T_s}{m}} dt \) and \( \beta \) is the absolute value of the slowest eigenvalue, that is a known function of \( \alpha \) and \( \epsilon \).

Now, let us suppose that there are gradients in the horizontal plane. The previous results make plausible a description in terms of the 2D density, \( n(r,t) \), 2D flow velocity, \( \mathbf{u}(r,t) \), and horizontal temperature, \( T(r,t) \). The evolution equations for these fields are assumed to be of the form

\[
\begin{align*}
\frac{\partial n}{\partial t} &= -\nabla \cdot (n\mathbf{u}), \\
\frac{\partial \mathbf{u}}{\partial t} &= -\mathbf{u} \cdot \nabla \mathbf{u} - \frac{1}{nm} \nabla \cdot \mathbf{P}, \\
\frac{\partial T}{\partial t} &= -G(n,T) - \mathbf{u} \cdot \nabla T - \frac{1}{n} (\nabla \mathbf{u} \cdot \mathbf{P} + \nabla \cdot \mathbf{q}),
\end{align*}
\]

where \( \mathbf{P} \) is the pressure tensor and \( \mathbf{q} \) the heat flux. In the low-density limit and to Navier-Stokes order, we assume \( P_{ij} = nT \delta_{ij} - \eta \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \delta_{ij} \nabla \cdot \mathbf{u} \right) \), and \( \mathbf{q} = -\kappa \nabla T - \mu \nabla n \), where \( \eta \) is the shear viscosity, \( \kappa \) the (thermal) heat conductivity and \( \mu \) an additional transport coefficient called diffusive heat conductivity that couples the heat flux with the density gradients and that is peculiar to inelastic collisions [2]. The unknown term \( G(n,T) \) describes the homogeneous evolution of the temperature. All the gradient contributions coming from the cooling/heating rate are neglected.

The system of equations (6)-(8) admits a homogeneous stationary solution, \( n(r,t) = n_s \), \( \mathbf{u}(r,t) = 0 \) and \( T(r,t) = T_s \). The two constants \( n_s \) and \( T_s \) must be related by Eq. (4) that has to be equivalent to \( G(n_s, T_s(n_s)) = 0 \). The objective now is to study if this state is linearly stable. To do that, it is convenient to introduce the dimensionless deviations of the fields around the homogeneous solution \( \rho \equiv \frac{n - n_s}{n_s} \), \( \mathbf{w} \equiv \sqrt{\frac{m}{2T_s}} \mathbf{u} \) and \( \theta \equiv \frac{T - T_s}{T_s} \), as functions of the dimensionless time scale, \( s \), and dimensionless space variable \( l \equiv n_s \sigma \mathbf{r} \). Let us also introduce the Fourier components of these functions through \( y_k \equiv \int dl e^{-ikl} y(l) \) and let us decompose \( \mathbf{w}_k \) into its parallel, \( \mathbf{w}_{k\parallel} \equiv \mathbf{w}_k \cdot \hat{\mathbf{k}} \), and transversal \( \mathbf{w}_{k\perp} \equiv \mathbf{w}_k \times \hat{\mathbf{k}} \) components (\( \hat{\mathbf{k}} \) is a unit vector perpendicular to \( \mathbf{k} \)). The evolution equation for the transversal component is \( \frac{\partial}{\partial s} \mathbf{w}_{k\perp} = -\mathbf{q}_{k\perp} \), that is decoupled from the rest of Fourier components, that verify

\[
\frac{\partial}{\partial s} \begin{pmatrix} \rho_k \\ w_{k\parallel} \\ \theta_k \end{pmatrix} = \mathbf{L} \begin{pmatrix} \rho_k \\ w_{k\parallel} \\ \theta_k \end{pmatrix},
\]

where the dimensionless transport coefficients, \( \tilde{\eta} \equiv \sqrt{\frac{\sigma}{2mT_s}} \eta_s \), \( \tilde{\kappa} \equiv \sqrt{\frac{m}{2T_s}} \sigma \kappa_s \), \( \tilde{\mu} \equiv \sqrt{\frac{m}{2T_s}} \sigma \mu_s \), have been introduced (the subindex \( s \) in the bare transport coefficients indicates that they are evaluated in the homogeneous stationary state). To obtain Eq. (11), the needed quantities \( \frac{\partial G(n_s, T_s)}{\partial n} \) and \( \frac{\partial G(n_s, T_s)}{\partial m} \) have been identified taking into account the analysis of the homogeneous
phase made previously. In effect, \( \frac{\partial G(n_\ast, T_s)}{\partial n} \) due to Eq. (10), while \( \frac{\partial G(n_\ast, T_s)}{\partial n} \) have been calculated using that \( G(n_\ast, T_s) = 0 \), so that \( \frac{\partial G(n_\ast, T_s)}{\partial n} = 2\beta n \frac{\partial G(n, T_s)}{\partial n} \).

The stability of the system depends on the properties of the matrix \( \mathbf{L} \) given by Eq. (10). The eigenvalues, \( \lambda \), of \( \mathbf{L} \) are the three roots of the following algebraic equation

\[
\lambda^3 + [\beta + (\bar{n} + \bar{k})k^2]\lambda^2 + [(1 + \beta\bar{n} + \bar{k}k^2)k^2 - \beta(\bar{\mu} - \bar{k})k^2]k^2 = 0
\]

Here, it is seen that a mode can vanish for a finite wavenumber, \( k = k_c \equiv \sqrt{\frac{\beta}{\bar{n} - \bar{k}}} \). In fact, it can be seen by general arguments that there can be only one unstable mode for small \( k \) [12]. This occurs only if the compressibility in the stationary state is negative, i.e. \( \frac{\partial \rho}{\partial n}(n_\ast) < 0 \), being \( \rho(n) \equiv nT_s(n) \), in which case it goes as \( \lambda \sim \sqrt{\frac{1}{2\beta}} \frac{\partial \rho(n)}{\partial n} k \) to first order in \( k \). For our model, the condition for the instability is fulfilled and the unstable mode goes as \( \lambda \sim \frac{1}{\sqrt{2}} k \). This mode becomes stable for \( k > k_c \) due to heat conduction (note that \( k_c \) depends also on \( \bar{\mu} \)). In Fig. 2, the real part of the eigenvalues of \( \mathbf{L} \) are plotted for \( \epsilon = 0.5 \) and \( \alpha = 0.9 \) as functions of \( k \).

The unstable mode for small \( k \) is more a question of “size” that of density and it is expected that a critical length can be identified in the experiments. Of course, the instability can be tuned by many other aspects such as friction with the walls, inelasticity of particle-wall collisions, or gravity to mention a few but, in our opinion, the essential ingredients have been identified. On the other hand, the coexistence between the solid and gas phases has not been treated as the formalism is no longer valid for high densities. Nevertheless, it seems that the simplicity of the model would allow to make progress in this direction.

The theory developed here can be generalized for moderated densities. At the Enskog level, position correlations can be taken into account in an effective way by multiplying all the terms excepting the wall contribution in Eqs (1) and (2) by the pair correlation function at contact, \( g_2(n_\ast) \). In this case, performing a similar analysis, the expression for the critical wavenumber is

\[
k_c = \sqrt{\frac{\beta g_2(n_\ast)}{\bar{n} - \bar{\mu}}} \left( 1 + 2n_\ast \frac{\partial \log g_2(n_\ast)}{\partial n} \right).
\]

We have performed MD simulations to check the validity of this expression. Concretely, we have taken \( \alpha = 0.9 \), \( \epsilon = 0.5 \) and two different densities, \( n_\ast\sigma^2 = 0.15 \) and \( n_\ast\sigma^2 = 0.3 \). For the first density and taking the approximate expression for \( g_2 \) given in [21], the theoretical prediction is such that the system is supposed to be unstable above a number of particles \( N_c \equiv \frac{2\beta n_\ast\sigma^2}{\log} \sim 1650 \). We have performed MD simulations finding that for \( N = 1300 \) and 1400 the system is stable, for \( N = 1700 \) and 1800 unstable, while it is hard to say anything reliable for \( N = 1500 \) and 1600 as the system fluctuates from the homogeneous to the inhomogeneous phase. In the second density, \( N_c \sim 620 \), and for \( N = 500 \) and 600 the steady state was observed to be stable, while for \( N = 800 \) and 900 the system developed the instability. For \( N = 700 \) no conclusion could be reached from the simulations. Hence, we can say that the theory predicts well the stability/instability of the system.

To sum up, we have introduced a simple model that allows to explain from a microscopic point of view the origin of the instability in Q2D granular systems. Essentially, the idea is that there is one mechanism that destabilizes the system in the steady state (negative compressibility) and another one that stabilizes it (dissipation due to heat conduction). For small gradients, the first mechanism dominates the second one, making the system unstable, while for large gradients, the perturbation decays faster and the system is linearly stable. The fact that the compressibility is negative can be understood from the particular way in which energy is injected in the vertical direction and transferred to the horizontal direction through collisions. Hence, the instability is more a question of “size” that of density and it is expected that a critical length can be identified in the experiments. Of course, the instability can be tuned by many other aspects such as friction with the walls, inelasticity of particle-wall collisions, or gravity to mention a few but, in our opinion, the essential ingredients have been identified. On the other hand, the coexistence between the solid and gas phases has not been treated as the formalism is no longer valid for high densities. Nevertheless, it seems that the simplicity of the model would allow to make progress in this direction.

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