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Spontaneous Formation of Vortex in a System of Self Motorised Particles

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Abstract. — We study a system of disks with inelastic collisions. Energy is given to the system via a force of constant modulus, applied on each particle in the direction of its velocity. This system shows a dynamical phase transition from a disordered system towards a system organized into a vortex when the dissipation is increased. The state equation of the disordered system is obtained by using kinetic theory arguments. We also show that the transition is similar to the kinetic-cluster transition observed in the cooling of a gas of inelastic particles.

1. Introduction

Some years ago, the kinetic theory has been extended to the study of the dynamics of granular systems [1-4]. The main difference between gases and granular media is energy dissipation during collisions. Thus either the energy of the granular media decreases with time, or energy must be supplied by a source to maintain the velocity fluctuations. This happens in flowing particles when potential energy is transformed into kinetic energy. Another way to put energy in a granular system is through the motion of boundaries, as in the so-called Brazil nut problem [5-7]. On an air table, thin particles move and rearrange permanently because of small scale heterogeneities: they receive energy from air flowing upwards through the porous table [8].

Recently, Vicsek et al. [9] have introduced a model of self-driven particles to describe biologically motivated interactions ("Molecular motors" [10]). In this model, each particle is driven with a constant absolute velocity and assumes the average direction of motion of its neighbours with some added noise. A kinetic phase transition from no transport to finite net transport is observed when the density of particles is increased and the noise is decreased.

The way we use here to introduce energy into a dry granular material drives the system in a steady state, with constant energy. The model that we consider consists of a two-dimensional

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assembly of disks with hard-core interactions in a container with fixed boundary conditions. It is studied using Molecular Dynamic simulations as described by Herrmann [11]. To introduce energy into the system, we apply a constant force on each particle, such as in schools of fish, or flying birds in formation. This force is in the direction of the velocity of the particle and its modulus is constant. It has been observed previously [12,13] that an inelastic gas exhibits a transition from a homogeneous regime towards a regime with long-range correlation of the velocities and positions when the energy dissipated during the collisions is increased. In our system, the correlation of velocities leads to a single vortex. Recently, Hemmingsson [14] used the same model simulated on a lattice gas and also found vortex formation. We show that a theoretical approach similar to that presented by Haff [1] can describe the system in the disordered homogeneous phase. The phase diagram and the origin of the instability are then discussed.

2. Description of the Model

Molecular dynamics is a method to study $n$-body problems by solving equations of motion. It was first used to study liquids [15]. More recently, it was used to study granular materials [11,16].

Let us consider a two-dimensional system of $N$ particles of mass $m$ and radius $R = 0.5$, in a square box of length $L$, with fixed boundary conditions. When two particles $i$ and $j$ overlap (i.e., their distance is smaller than the sum of their radii) three forces [11] act on particle $i$:

i) an elastic restoration force

$$f_{el} = Y m(r_{ij} - 2R){\bf n}$$  \hspace{1cm} (1)

where $Y$ is the Young modulus normalized by the mass, $m$ the mass of the particle, $r_{ij}$ the distance between the two overlapping particles, and ${\bf n}$ the unitary vector built on $r_{ij}$ pointing from $i$ to $j$;

ii) a dissipation due to inelasticity of the collisions

$$f_{diss} = -\gamma_n m(V_{ij}.{\bf n}){\bf n}$$  \hspace{1cm} (2)

where $\gamma_n$ is a phenomenological dissipation coefficient in the normal direction and $V_{ij} = V_i - V_j$ is the relative velocity of particles $i$ and $j$;

iii) a shear force friction which is chosen as

$$f_{shear} = -\gamma_s m(V_{ij}.{\bf s}){\bf s}$$  \hspace{1cm} (3)

where $\gamma_s$ is a phenomenological dissipation coefficient and $s$ the unitary vector obtained by rotating $n$ by $90^\circ$.

During collisions with the walls, the force applied on the particles is similar to that used for interparticle collisions. It means that collisions with walls also dissipate energy. Particles are not allowed to rotate, and no Coulomb friction is considered. In the following, we will take $\gamma_s = \gamma_n = \gamma$. As Hook's law is used for the restoration force, the energy restitution coefficient of collisions, $\epsilon$, does not depend on the relative velocities of the colliding particles. An exact relationship between $\epsilon$ and $\gamma$ can be derived from the equation of motion. This relationship does not depend on particle velocity and can be written as follows:

$$\gamma \propto (\pi^2 + \ln^2 \epsilon)^{-0.5} \sqrt{V} \ln \epsilon$$  \hspace{1cm} (4)
A first-order expansion of this formula when $\epsilon$ is close to 1 gives $\gamma \propto 1 - \epsilon$.

An external driving force is applied at every time step on each particle to put energy into the system. The modulus of this force is constant and its direction is given by the velocity direction; so the force applied on the $i$th particle can be written as:

$$F_i = ma \frac{V_i}{V_i}$$

where $V_i$ is the velocity vector of the $i$th particle, $V_i$ the modulus of this vector, and $a$ is the "Force factor". The modulus of the acceleration does not depend on the mass or the velocity of the particle. Trajectories are calculated using a third order predictor-corrector method [17].

For low packing fraction (lower than 0.5), the initial positions of the particles are chosen randomly by an R.S.A (Random Sequential Adsorption) algorithm [18]; for packing fraction larger than 0.5, as the R.S.A. algorithm can no longer be used, the centers of the particles are initially situated on the nodes of a square lattice. In both cases, the initial velocities of the particles are randomly chosen. In order to let the system reach equilibrium, measurements are started after about $10^5$ time iterations (ten seconds). During each simulation, the total energy of the system (kinetic energy and elastic energy) is recorded. In order to characterize the global motion of particles we have used the kinetic momentum defined as:

$$M = \sum_{i=1}^{N} OM_i \wedge V_i$$

where $OM_i$ is the vector linking the center of the $i$th particle to the center of the box. If a vortex appears in the system, the time average of $M$ has a finite value. For a disordered system, the time average of $M$ will be zero. Thus the kinetic momentum can be used as an order parameter to characterize a single vortex.

3. Kinetic Regime - Theoretical Results

One of the fundamental assumptions of the kinetic theory is that of complete molecular chaos. This means that there are no correlations between the velocities of the individual colliding particles. In our system, we assume that there are neither velocity nor position correlations. Thus, we can apply a modified kinetic theory to find a state equation of the system. The principle is to consider that the system is in a steady state with a balance between the input energy and the energy dissipated by collisions. Both energies can be calculated, and this leads to an equation giving the mean square velocity as a function of the packing fraction $C$, the force factor $a$ and the energy restitution coefficient $\epsilon$ of collisions.

The energy given per time unit to the $i$th particle by the force factor is:

$$\frac{dW_i}{dt} = maV_i$$

By averaging over the whole system, the mean energy given per particle and per time unit can be written as:

$$\frac{dW}{dt} \propto maV$$

where $V$ is some average over the particle velocities. We have verified that the velocity distribution is never far from a Maxwell distribution, so that all averages of velocities of the particles are proportional to each other. As in the following, we use proportionality instead of strict
equality, $V$ can be the mean square velocity, as well as the most probable velocity. In the same way, we do not distinguish between mean velocity of the particles and mean relative velocity of two particles.

To calculate the dissipated energy, we neglect effects of the walls and consider that energy is dissipated only by collisions between particles. The energy dissipated per particle and per time unit is proportional to the number of collisions per time unit and to the average energy dissipated at each collision.

For a two-dimensional ideal gas, the number of collisions for one particle per unit of time is of the form:

$$n \propto \frac{V}{l}$$  \hspace{1cm} (9)

where $l$ is the mean free path of the particles. To apply this relation to a granular medium, we have first to assume that the contact time is very small compared to the time of free flight. This is clearly true in the case of low packing fraction and high restitution coefficient. In the case of our granular system, as the packing fraction is high, the size of the particles cannot be neglected in front of the mean free path of molecules in an ideal gas. Thus we write the mean free path in the following form:

$$l = \lambda - \Gamma(R)$$  \hspace{1cm} (10)

where $\lambda$ is the mean free path of a molecule in a ideal gas and $\Gamma(R)$ is a perturbation taking into account the reduction of the mean free path due to the size of the particles. As the packing fraction $C$ is an easily accessible quantity in a granular medium, we use the following relationship for $\lambda$:

$$\lambda = \frac{L^2}{N\sigma} = \frac{\pi R}{2C} \text{ with } C = \frac{N\pi R^2}{L^2}$$  \hspace{1cm} (11)

$\sigma = 2R$ is the section of collision. If we assume that there are only frontal collisions, one could expect $\Gamma(R) = 2R$. Non-frontal collision leads to a value of $\Gamma(R) < 2R$. Assuming that there are only binary collisions and that the impact parameter is a random variable, an exact calculation gives $\Gamma(R) = \frac{\pi R}{2}$. In a more general case (multiple collisions), as a first approximation we take $\Gamma(R)$ proportional to the radius $R$ of the particles. Then we write:

$$l \propto \left(\frac{1}{C} - k\right)R$$  \hspace{1cm} (12)

where $k$ is a dimensionless constant. When the packing fraction approaches the value $C_0 = 1/k$, $l$ tends to 0.

The energy dissipated during one binary collision is also proportional to $(1 - \epsilon)mv^2$, where $\epsilon$ is the energy restitution coefficient. Using the energy dissipation coefficient $d = 1 - \epsilon$, we find that the dissipated energy per particle and per time unit is proportional to the cube of the mean velocity divided by the mean free path.

$$\frac{dW}{dt} \propto ndmV^2$$  \hspace{1cm} (13)

$$\frac{dW}{dt} \propto m\frac{d}{l}V^3$$  \hspace{1cm} (14)

A similar result has been obtained by Haff [1] using a similar approach. In the case of correlation of motion in the system, like for flowing particles, the same computation can be done, replacing $V$ by the fluctuation of velocity around its mean local value. For our system, as all particles
have the same mass and size and by considering the balance between the dissipated energy and the input energy, we find the following equation of state for the disordered steady state:

\[ V^2 \propto \frac{a}{d} \left( \frac{1}{C} - k \right) R \]  

(15)

4. Kinetic Regime - Numerical Results

In Figure 1, we have plotted in logarithmic scale the total energy \( E \) of the system versus \( \gamma \) for different values of \( a \), and given values of \( L \) and \( N \) (i.e., \( C \)). As \( \gamma \propto (1 - \epsilon) \), \( d \) is proportional to \( \gamma \) when \( d \) is close to zero. We have verified that this approximation is valid for the results shown below. Therefore we will use \( \gamma \) instead of \( d \) in the following. For low values of \( \gamma \), the variations of \( E \) are linear with the same slope \((-1)\) for all \( a \), \( L \) and \( C \). In agreement with the theoretical state equation (15), \( E \) is proportional to \( 1/\gamma \) and also to \( a \). Above a certain value \( \gamma_c \) of \( \gamma \), the energy is larger than the theoretical one: we will see below that this is due to a transition of the system to a vortex regime.

In order to compare all results, we have plotted in Figure 2 a normalized energy per particle \( \frac{1}{C} \) versus \( \gamma \) for different values of \( a \), \( d \), \( N \) and \( L \) for \( \gamma < \gamma_c \). The normalized energy \( E_n \) is defined as:

\[ E_n = \frac{1}{N} \frac{E}{d} \]  

(16)

A very good agreement is found between the theoretical equation of state (represented by the straight line) and the numerical data. The value obtained for \( C_0 = 1/k \) is \( 0.82 \pm 0.01 \). It is not compatible with that calculated by assuming that there are only binary collisions (\( C_0 = 1 \), see above). Surprisingly, it is the same density as that of the 2D Random Close Packing (R.C.P.).
Above this density long-range correlations appear in the positions of particles \([19]\). So the model predicts that the system has no velocity fluctuations around the local average when it reaches such a packing fraction.

5. Phase Transition - Numerical Results

One can notice in Figure 1 that while \(\gamma\) increases above the value \(\gamma_c\), the energy becomes larger than that calculated by the kinetic theory. This is due to a phase transition from a disordered system \((\gamma < \gamma_c)\) to a system organized into a vortex \((\gamma > \gamma_c)\). The kinetic momentum \(M\) is used as a parameter to characterize the presence of a single vortex. One can see in Figure 3 that \(M\), which fluctuates around 0 for \(\gamma < \gamma_c\), decreases steeply to a negative value (constant in time and depending of \(L, a, \gamma\) and \(C\)) when \(\gamma\) is increased above \(\gamma_c\). Figure 4 gives a snapshot of a system below \(\gamma_c\), with no correlation of velocity or position, \(M\) is a white noise of zero average. Figure 5 shows the same system above \(\gamma_c\): locally, the velocities of the particles all point in the same direction. The global motion is a vortex and \(M\) fluctuates in time around a constant (non-zero) value. The packing is not homogeneous, the density being larger near the boundaries than in the center of the cell.

From the values of \(\gamma_c\) obtained in many simulations, with different values of \(a, L,\) and \(N\), we have plotted (Fig. 6) in the plane \((\gamma, 1/C)\) the lines separating the vortex regime (above) from the homogeneous regime (below), for three values of \(L\). It appears that the transition lines do not depend on \(a\). On the contrary, the transition strongly depends on the size of the system: the larger the box, the lower \(\gamma_c\). For very small values of \(C\), no transition is observed in the studied range of \(\gamma\); the system is homogeneous. Then when \(C\) increases, the transition curves show a minimum for a value of \(C\) close to 0.6 increasing slightly with \(L\).

In a gas of inelastic particles, a local increase of the packing fraction \(C\) increases the collision frequency and thus the local dissipation of energy (dissipation of the relative velocity). The pressure is proportional both to \(C\) and to the velocity fluctuations. When the density of
Fig. 3. — Linear plot of the kinetic momentum $M$ versus $\gamma$ for $L = 15$, $a = 5$, $C = 0.45$. $\gamma$ is increased from 1 to 11 and then decreased to 1.

Fig. 4. — Snapshot of a system of 400 particles in the disordered phase ($C = 0.5$, $a = 1$, $\gamma = 1$). The size of the box is $L = 25$. The circles represent the particles, the lines represent the velocity vectors.
Fig. 5. — Snapshot of a system of 400 particles in the vortex regime \((C = 0.5, \alpha = 1, \gamma = 5)\). The size of the box is \(L = 25\). The circles represent the particles, the lines represent the velocity vectors.

Fig. 6. — Transition lines from a disordered system to a vortex regime in the \((\gamma, 1/C)\) plane for different sizes \(L\), \(\alpha\) being between 0.1 and 1.

particles locally increases, if the dissipation is large (\(d\) large), there will be a decrease of the pressure in that place. The flux of particles will then go from low packing fraction and high energy areas to high packing fraction and low energy areas amplifying the density variation and leading to the formation of a “cluster”. This is the origin of the transition from the “kinetic
regime" to the "cluster regime" in the cooling of a gas of inelastic particles as described by Goldhirsch and Zanetti [12] and McNamara [13]. The velocity of the center of mass of a cluster is not modified by the collisions of particles inside the cluster, and in our case the center of mass of a cluster is accelerated by the force. This mechanism tends to decrease velocity fluctuations in a certain neighbourhood, and amplify the macroscopic motion. This is also the mechanism explaining the dynamical phase transition observed by Vicsek et al. [9] (the averaging of velocity directions in the Vicsek model can be compared locally to the cooling of a granular medium). The appearance of long-range self organized motion therefore seems to be a general property of dissipative interactions. Another argument in favor of the relation to the kinetic-cluster transition is the shape of the transition lines. For $C < 0.6$, we have $\gamma_c \propto 1/L^2 C^2$. This is the limit of the stability of the heat mode (homogeneous cooling) of a gas of inelastic particles as given by McNamara [20] who also found a particular behaviour for high packing fractions.

6. Conclusion

Increasing the dissipation in a granular medium, we have observed a transition from a homogeneous regime to a vortex regime. This appears to be similar to the kinetic-cluster transition observed by McNamara [13]. In our case, a vortex is the only possible steady motion with long-range order compatible with fixed boundary conditions, as compared to the two streams found by McNamara [20] when periodic boundary conditions are applied. Some higher order modes can be obtained in a rectangular box; nevertheless, they are not stable: depending on the initial conditions we can have two metastable vortices, but after a while, one of the vortices stretches out, and its motion becomes faster and faster, the other vortex becomes smaller and smaller, its packing fraction increases, and its motion slows down (the viscosity increases with the packing fraction). The system then evolves towards one elongated vortex filling the entire system. The energy of this vortex is higher than the energy of the two small vortices. The instability of high-order modes and the independence of the transition from the force factor $a$ (taking the temperature proportional to the energy) seem to show that this instability is different from the Rayleigh-Bénard or other classical hydrodynamic instabilities under gradient.

This model also gives information on the kinetics of dissipative gases. The R.C.P limit appears to be important for dynamical properties. It is the maximum packing fraction above which uncorrelated motion is no more possible. It is also the limit where the viscosity increases steeply because of geometrical effects. This probably explains that $d_c$ increases for $C > 0.6$.

Some different forces could be studied. A force depending on the local packing fraction must modify the transition. Adding a noise to the force could also be interesting.

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