Effects of Attractors on the Dynamics of Granular Systems

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Failing to satisfy Liouville's theorem, the dynamics of granular materials is affected by the attractors in their phase spaces. Motion of inelastic hard disks in a thin pipe with energy sources at both ends of the pipe is simulated and the statistical steady state is studied. We investigate the probability distribution function of the spacing l between neighboring particles, and find that the attractors can lead to a phase of the cluster of particles with structures different from that of an ideal gas. [S0031-9007(98)05933-X]

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Granular materials are excellent for studying the dynamics of dissipative systems. Generally, they consist of macroscopic grains which do not interact with one another except when they collide inelastically. Naively, one would expect that these grains are a whole bunch of loose sand, which behave like an ideal gas with some modification due to the energy dissipation. However, they exhibit rich dynamical behaviors. One of the most interesting behaviors is the collective motion of these grains, such as convection, surface wave pattern formation, etc.; see Ref. [1] and the references therein. According to the second law of thermodynamics, an isolated system tends to reach maximum disorder. However, in granular materials, energy dissipation creates order out of the collection of loose grains.

In this Letter, we investigate one of the consequences of energy dissipation, the attractors in the phase spaces of granular systems. One of the cornerstones of the classical kinetics and hydrodynamics theories, Liouville's theorem states that the phase space volume is a conserved quantity [2]. However, Liouville's theorem is only valid for conservative systems. For dissipative dynamical systems, phase space volume is no longer a conserved quantity, and, consequently, attractors appear in the phase space [3]. These attractors may change the structure of the collection of grains. And so a proper understanding of these attractors and the resulting structure is very important for a correct theory of the dynamics of granular materials.

For the hard sphere model of granular systems with strong enough inelasticity, these attractors can lead to a finite time singularity, inelastic collapse [4–7]. During inelastic collapses, several particles undergo an infinite number of collisions in a finite time interval. At the moment of singularity, the spacing between neighboring particles vanishes. In one dimension, the velocity differences among collapsing particles also vanish, and these particles stay together after the singularity. While in higher dimensions, this is generally not the case—only the radial relative velocities between neighboring particles vanish, while the tangential relative velocities remain finite. As a result, collapsing particles generally separate from one another after the singularity.

There are controversies about the effects of inelastic collapses. Since inelastic collapses are short time events, it is not clear whether they have any significant influences on the long term behavior of the system. If, after being averaged over a long time interval, the effects of inelastic collapses are negligible, they are not relevant to any hydrodynamics description of granular systems. However, we will show that the attractors manifested by inelastic collapses lead to a structure of the grains different from that of an ideal gas, and so they are important for the long term behavior of the systems.

Here, we study a two-dimensional system of identical grains confined in a thin pipe (Fig. 1). The width of the pipe is set so that two grains cannot pass each other. Thus, the motion of grains is two dimensional to ensure ergodicity, while at the same time we can order these grains. The two side walls are periodic—after leaving one side wall a particle comes back through the other. The two end walls are energy sources, and are kept at the same temperature. For details, see Ref. [8].

We use the simplest collision model—after a collision, the normal relative velocity changes sign, and decreases by a factor of the restitution coefficient r, with $0 < r < 1$. In the collision, the other components of the velocities are unchanged.

Simulations are for 100 particles. Statistical analysis is done for the statistical steady state. To avoid complications due to different geometrical factors we carry out our numerical calculations only for systems with extremely high density, where the typical spacing between neighboring particles is about 2% of the radius of a particle, or for systems with extremely low density, where the spacing at the highest density region of the system is about 10 times the radius. For the high density cases, the critical value of the coefficient of restitution for inelastic collapse r_c is

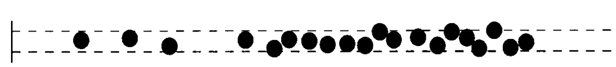

FIG. 1. A snapshot of the thin pipe system. The periodic side walls are indicated by dashed lines. The two end walls are energy sources kept at the same temperature. The coordinate system is set up so that the x axis is along the pipe.

about 0.94, while for the low density cases, it is about 0.92. We carry out simulations at these extreme values of r to investigate the structure of the cluster of grains when they nearly collapse. Here we only show plots for the low density systems, because the essential dynamical characters are the same for the high density systems.

An interesting quantity which serves as a signature for the structure is the spacing l between neighboring particles. For a system of elastic particles in equilibrium, the distribution for l is a simple exponential law,

$$P(l)\,dl = \frac{1}{\lambda}\exp\left(-\frac{1}{\lambda}\right)dl\,, \tag{1}$$

where λ is the mean free path. It can be derived from basic statistical considerations as follows. For simplicity, let us consider N point particles on a circle, although the following calculation can easily be modified for higher dimensions. Let us divide the circumference into M equal length segments, with M very large. Suppose particle i is in one of the segments. Let us calculate the probability that there are m empty segments between particle i and particle $i+1$. Since the system is in equilibrium, the entropy reaches its maximum. Equivalently, we can assume each state has the same probability weight. When there are m empty segments between particle i and particle $i+1$, there are $M-m$ segments available to other $N-2$ particles, so its probability is proportional to the number of different states, which is

$$\frac{(M-m)^{N-2}}{(N-2)!} \propto e^{-(N-2)m/M}\,.$$

Hence the spacing distribution for a state in equilibrium is in the linear exponential form of (1).

Since our system is not strictly one dimensional, we need to elaborate on the meaning of spacing. The motion of the particles is two dimensional, and the periodic side walls make the distance traveled in the y direction ambiguous. So we consider only the spacing in the x direction. Define $l_i \equiv x_{i+1} - x_i - l_{\min}$; to take into account the finite size of particles, we put a modification into the definition, the minimum distance between the centers of neighboring particles, $l_{\min} = \sqrt{(2R)^2 - (W/2)^2}$, where R is the radius of a particle, and W is the width of the pipe.

In our simulations, we do not observe a probability distribution in the linear exponential form of (1) for spacings between any neighboring particles when r is very close to unity. But when r gets smaller, the form of the distribution changes. Near the boundary, the distribution is still very close to the linear exponential form, while inside the system, there is an obvious deviation from it. When r is very close to r_c, the distribution of spacing between two central particles l_0 is of the form (Fig. 2)

$$P(l_0) \propto \exp(-\sqrt{l_0/\lambda})\,. \tag{2}$$

This distribution is not simply a result of the strong inhomogeneity, because the distribution near the boundary is in the old linear exponential form where the inhomogeneity is even stronger due to larger energy flux. It suggests, inside the cluster, a structure different from that of an ideal gas. As we will see from the following calculation, this structure is a result of the attractors in the phase space of the system.

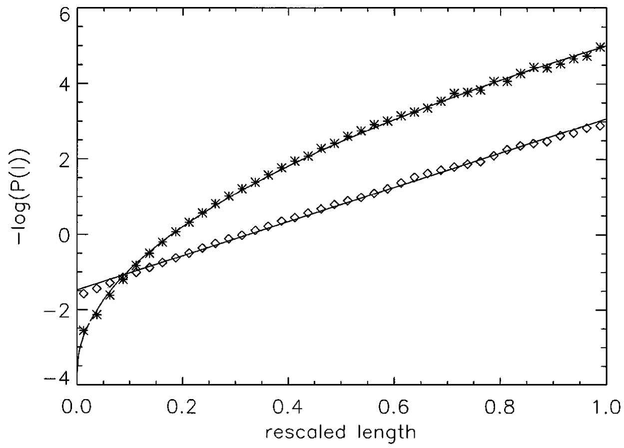

FIG. 2. The probability distribution for the spacing between two neighboring particles for a low density system with 100 particles and $r = 0.94$. The abscissa is rescaled length. ◇ symbols are for distribution of spacing between two neighboring particles which are very close to the end walls, the distribution is in the linear exponential form (1). $*$ symbols are for distribution of spacing between two central particles; the fitting curve is in the form of a constant plus the square root of the spacing, corresponding to Eq. (2).

Because the two dimensional motion of grains is ergodic [8,9] it is reasonable to assume the above derivation which leads to (1) still holds to some extent. Now let us consider the particularities of situations for strong inelasticity, for which there are strong attractors in the phase space. When particles move towards the attractor, the size of the whole cluster is decreasing, while when particles leave the attractor, the size of the cluster is increasing. So the characteristic length scale is not fixed, and consequently λ in (1) changes with time.

Let us consider the probability distribution function (PDF) for the characteristic length scale. The distance between two far apart particles can be used to describe this length scale. First, for elastic particles, we still use the one dimensional model from above. Let us study the distance between two particles which have N_1 particles between them. Still supposing there are m segments between these two particles, then its probability is proportional to the number of states,

$$\frac{M^{N_1}(M-m)^{N-2-N_1}}{N_1!\,(N-2-N_1)!}\,. \tag{3}$$

The maximum is reached when $m = m^* \equiv MN_1/(N-2)$. When both N_1 and $N - N_1$ are big, m nearly always takes values very close to m^*. For a system of elastic particles, the length scale is fixed, taking a value corresponding to m^*. The changes in the distance are small thermal fluctuations, which decrease with increasing system size. This distribution is shown in Fig. 3. The shape of the dashed line in the figure does not show a sharp distribution for a fixed length. This is because of big thermal fluctuations due to the limited number of particles.

Now let us consider the situation when r is very close to the critical value of collapse. The solid line in Fig. 3 describes the distance between two particles which are positioned symmetrically about the center with 38 particles between them. This distance describes the size of the cluster of particles, although there are no clear boundaries for the cluster. Since under this circumstance the system is very nonuniform, the length scale is different for different parts of the system, so the distance described in Fig. 3 can be taken only as an approximate indicator of the length scale. We see the PDF is in the form of an exponential function modified by some power law near the origin.

There are also big thermal fluctuations for the PDF shown by the solid line. But we can assume that the shape of PDF of thermal fluctuations around a fixed length scale, shown as the dashed line in Fig. 3, is the same for all length scales. Furthermore, this PDF of fluctuations decreases rapidly when the distance deviates from the distance corresponding to the maximum probability. Then the exponential distribution shown as the solid line in Fig. 3, which is essentially the superimposition of all the "distribution packages," indicates an exponential PDF for the length scale.

The PDF of the length scale shows how strong these attractors are. For quasielastic situations, when we expect these attractors are rather weak, the PDF of the length scale is very close to the one for elastic particles. Only when r is small, or when N is big, we see a significant deviation from the elastic distribution, as a result of the strong attractors in these situations.

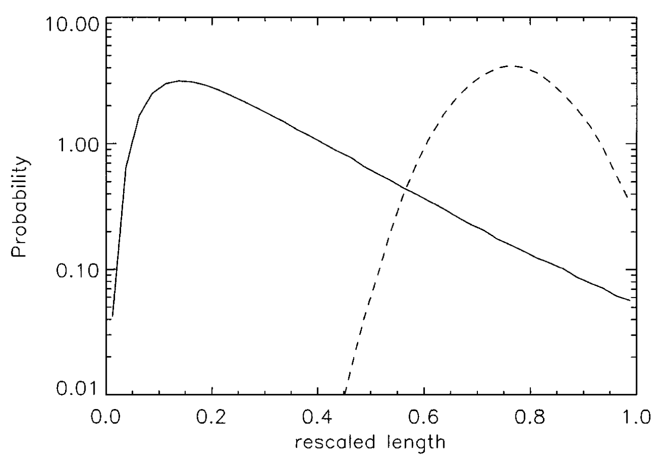

FIG. 3. The probability distribution for the distance between particle 31 and particle 70, which have 38 particles between them. The system is in low density regime with 100 particles. The abscissa is rescaled length. The dashed line is for elastic particles, $r = 1$. The solid line is for $r = 0.94$, giving an exponential function modified by some power law near the origin as the PDF for the length scale when the particles nearly collapse.

We can understand this PDF of the length scale in the following way. In Eq. (3), there are two contributions: First, the thermal motion of internal particles, which are particles between the two particles, tries to expand this distance, and makes the probability rather small for small value of this distance; second, the thermal motion of outside particles tries to suppress this distance, and makes the probability small for big value of this distance. When these two factors are in balance, the probability reaches its maximum. However, when the attractors are very strong, the thermal motion of internal particles are suppressed, and only the thermal motion of outside particles is important. This leads to an exponential distribution of the distance just as if there were no internal particles, corresponding to (1).

There are several mechanisms which can contribute to the power law of the PDF near the origin as shown in Fig. 3. First, as mentioned above, the thermal motion of internal particles can contribute in such a form as to reduce the probability when the distance is very small.

Another mechanism is inelastic collapse. When particles are collapsing, the length scale, velocity scale, and time interval scale all decay exponentially with the cycle number n [6]. Suppose they are, respectively,

$$\lambda = \lambda_s a^n, \qquad v = v_s b^n, \qquad t = t_s (a/b)^n.$$

Then

$$P(\lambda) \propto t_s (a/b)^n \propto a^{n(1-\log b/\log a)} \propto \lambda^{1-\log b/\log a},$$

where a and b depend on r. So the PDF is a power law when particles are collapsing, or, equivalently, for very small λ.

Also the situation for very small λ is complicated by the finite size of particles for low density systems, or by the geometrical factors for high density systems. But we believe the solid line in Fig. 3 reflects the essential characteristics of the PDF.

We can now calculate the PDF for the spacing between two central particles. Since the motion of particles is still random enough, the spacing between these two particles l_0 obeys a distribution $\frac{1}{\lambda}\exp(-\frac{l_0}{\lambda})$, where λ is a characteristic length. Because of the attractor, the characteristic length changes, and let us assume it has a distribution in the form $\lambda^\nu \exp(-\frac{\lambda}{\alpha})$. Then we have

$$P(l_0) \sim \int_0^\infty \lambda^{\nu-1} \exp\left(-\frac{\lambda}{\alpha} - \frac{l_0}{\lambda}\right) d\lambda \,. \tag{4}$$

From the integral

$$\frac{1}{\sqrt{\pi}} \int_0^\infty \frac{d\lambda}{\sqrt{\alpha\lambda}} e^{-(\lambda/\alpha)-(l_0/\lambda)} = e^{-2\sqrt{l_0\alpha}},$$

we know when $\nu = 1/2$, $P(l_0)$ calculated from (4) is exactly in the form of (2). Even when ν takes some other value, it only makes some modification to $P(l_0)$ for small l_0, and (2) still describes the PDF for most values of l_0.

From above we see that, although inelastic collapses are short time events, they manifest the attractors in phase space which change the structure of the cluster of particles. The PDF for the spacing between two central particles l_0 changes from (1) for $r = 1$, the elastic case, to (2) for $r \approx r_c$, the near collapse case. This change of the PDF is a continuous function of r; i.e., if the PDF is of the form of $\exp[-(l_0/\lambda)^\gamma]$, then γ is a continuous function of r. Also, for $r \approx r_c$, this γ is a continuous function of the position of the two particles in the system, it changes from 1 for particles near the boundary to $1/2$ for central particles. So if there is a phase transition, it can only be a smooth one. Also, the meaning of "phase transition" is ambiguous when we do not have the luxury of taking thermodynamics limit.

We also notice that r_c depends on the system size. This show the character of the attractors not as a result of local motion of grains, but as a result of collective motion of the whole system. It is related to the instability described in [10]. The numerical results shown here are for $r \geq 0.94$, which is still quite close to unity. For even smaller r and the same system size, the whole system, save maybe several particles at the boundaries, will be in a different phase characterized by the attractors. An investigation of the velocity PDF of granular system using the Boltzmann equation is carried out in [11]. However, we would argue that the validity of the Boltzmann equation for granular materials still needs to be clarified [2].

These attractors are intrinsic property of the dynamics of granular systems. When one is studying such intrinsic properties, one should try to avoid or separate effects from boundary and initial conditions. For example, when one simulates the free evolving process of a granular system from some homogeneous initial state with Gaussian velocity distribution of the grains, the agreement between hydrodynamics theory and numerical results for some early time of the evolving process may not suggest that the hydrodynamics theory captures the essential dynamical properties of the system. To capture such properties, one has to wait a long enough time in the simulation for the initial condition to be "forgotten." Similarly, for granular systems under external forcing, it is important to distinguish the effects of the forcing from those of intrinsic dynamics. We see this in Fig. 2, where the attractors only have effects far inside the system, while near the boundary the effects of forcing dominate the dynamics.

Last, we want to mention that the distribution (2) is a combined result of the ergodic motion and attractor effects. For strict one dimensional situations, there are strong attractor effects. However, the motion of particles in one dimension is not ergodic [12,13], so the distribution (2) is not observed.

As to the relevancy of the pipe model to the practical granular dynamics problem, we want to point out that it is the simplest situation which can show hydrodynamic behavior. In an unpublished work, Kadanoff, Ban-Naim, Grossman, and Zhou showed that the pipe system behaves essentially in the same way as the two dimensional system in [9]. Also see [14] for interesting work done for the pipe system.

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