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Inelastic collapse in two dimensions

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Molecular dynamic simulations show that a two-dimensional gas of inelastic disks, started from random initial conditions, has a finite time singularity in which a group of particles spontaneously forms a straight line. The inelastic disks then collide infinitely often in a finite time along their joint line of centers. The upshot of this process is a multiparticle collision that occurs through the accumulation of an infinite sequence of binary encounters.

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In this paper we present the results of recent molecular dynamic simulations of a two-dimensional granular medium. This is a gas of inelastic disks in which interactions occur only through collisions. The inelasticity is modeled with a coefficient of restitution $0 \leq r \leq 1$ that reduces the relative velocity along the line of centers so that momentum is conserved and kinetic energy is dissipated [1]. The classical hard core gas is the special case $r=1$. The granular medium is at once a useful idealization in many applications and a fundamental model in dissipative statistical mechanics.

Consider a granular medium that begins in an initial state of uniform density with a Maxwellian distribution of velocities. (This initial condition is established by running the simulation with $r=1$ for several hundred collisions per particle.) The medium then "cools" as the collisions dissipate the kinetic energy of the initial condition [2]. Recent work [3,4] has established that the cooling granular medium does not remain spatially uniform: the state of uniform density is unstable so that clusters and voids form throughout the gas.

It is essential to draw a clear distinction between *clustering* and *collapsing* in a granular medium. By clustering we mean that the density of the granular medium spontaneously becomes nonuniform as described in the previous paragraph. The term collapse refers to "inelastic collapse" which is a finite time singularity previously documented only in one dimension [3,5]. In one-dimensional inelastic collapse a group of particles moving on a line collides infinitely often in a finite time so that the interparticle spacing becomes zero and all of the kinetic energy in the center of mass frame is dissipated. The result of inelastic collapse is that the particles come into contact without interparticle forces or cohesion. By contrast, in a cluster the particles are close together, but they are not in contact.

In one dimension, inelastic collapse is tolerably well understood and it is possible to estimate the minimum number of particles $N_{\text{min}}(r)$ required to form the finite time singularity [3,5]. When $r \ll 1$, so that the system is almost inelastic, only small numbers of particles are involved. For instance, if $0<r<7-4\sqrt{3}$ then the collapse only takes three particles; if $7-4\sqrt{3}<r<3-2\sqrt{2}$ then collapse requires at least four particles. The elastic limit is singular in the sense that $N_{\text{min}}(r) \sim \ln[4/(1-r)]/(1-r) \to \infty$ as $r \to 1$.

One might suspect that inelastic collapse is a pathology of one dimension. But the first result of this paper is that collapse also occurs in two dimensions and does so by recapitulating the one-dimensional phenomenology. Figures 1 and 2 show the results of the "inelastic few-body problem." We have three or four inelastic disks moving in a doubly periodic domain. In both cases $r=0.05<7-4\sqrt{3}$ and the disks occupy $\frac{1}{4}$ of the area. Figures 1 and 2 show the configuration of the disks at the time of the singularity [6]. Remarkably, one finds that the disks are roughly in a line. Thus in two dimensions, three or four inelastic disks can collide infinitely often in a finite time by bouncing back and forth along their joint line of centers. Figure 3 provides a more quantitative illustration by showing the number of collisions as a function of elapsed time in ten simulations. The singular events are the vertically rising segments which terminate seven of the ten simulations.

We performed 50 simulations with $N=3$ particles, $r=0.05$ and solid fraction $\nu=\frac{1}{4}$. Twenty-one realizations were stopped in finite time by inelastic collapse detected by the separation criterion explained in [6]. The other 29 real-

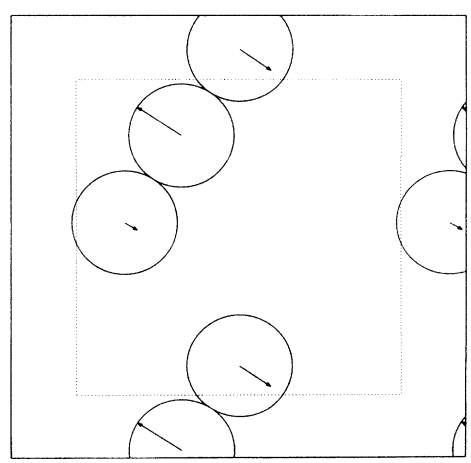

FIG. 1. Three inelastic disks ($N=3$) in a doubly periodic domain at the time of collapse. One period is contained within the dotted square. The solid fraction $\nu=\frac{1}{4}$ and $r=0.05$.

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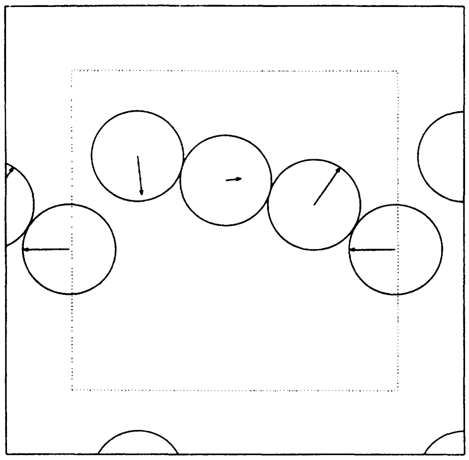

FIG. 2. Four inelastic disks ($N=4$) in a doubly periodic domain at the time of collapse. As in Fig.1: $r=0.05$ and $\nu=\frac{1}{4}$.

izations ran till $C/N=30$. In a second suite of 50 realizations with $N=4$ particles (once again $r=0.05$ and $\nu=\frac{1}{4}$) 41 realizations were stopped by inelastic collapse while the other 9 ran till $C/N=30$. In Figs. 1 and 2, and in all of the other singular events, one finds that the particles are arranged in a rough line. In most of the cases with $N=4$ this line contains only three of the four particles. But in a few instances (e.g., Fig. 2) the line involves all four particles.

In Figs. 1 and 2 the velocities transverse to the line of centers are not zero so that in two dimensions the singularity does not dissipate all of the kinetic energy in the center of mass frame of reference. In fact, in the final stages of the singularity there is very little energy dissipation because the relative velocity of collision is going to zero exponentially with the total number of collisions. If one could "pass through the singularity" then the transverse velocities in Figs. 1 and 2 would break up the line. Our collision based

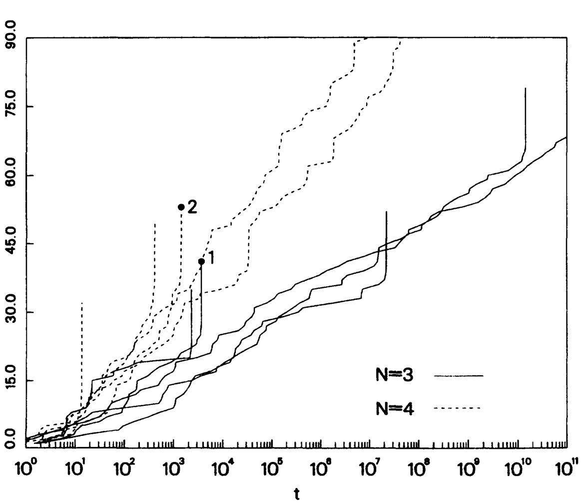

FIG. 3. The cumulative number of collisions as a function of elapsed time in eight simulations. The configurations shown in Figs. 1 and 2 are the heavy dots labeled "1" and "2."

computational strategy [7] cannot proceed past this singularity and capture the ensuing dispersal of the line. However this is not a fault of the numerical algorithm because the computation attempts to represent a singularity that is a true consequence of the idealized model defined in the first paragraph of this paper. In this classical model there is a collision rule for only *two* particle interactions. Inelastic collapse means that *three* (or more) particle collisions occur in finite time. The many-particle interaction occurs through the accumulation of an infinite sequence of two particle collisions as shown in Fig. 3. Thus the idealized model, with only a binary collision rule, becomes undefined at the time of the first singularity.

Inelastic collapse is a pathology of an idealized mathematical model. We hope that analyzing this singularity will help understand the behavior of real granular systems and we speculate that inelastic collapse is one route by which cohesionless grains can come into contact and develop long range position and velocity correlations. In a real granular medium this process does not require an infinite number of collisions, but merely a very large number. In this qualified sense the mathematical singularity identified by the idealized hard core model is an approximation of a physical phenomenon. A remaining issue is the "regularization" of the hard core model so that molecular dynamic simulations can advance through the singularity. But it is also essential to document the singularity itself, and this is the focus of the remainder of this paper.

It is interesting that in the kinetic theory of elastic ($r=1$) hard spheres the calculation of the short time or high frequency behavior of the scattering functions requires the resummation of a sequence of three body recollision events which occur in an infinitesimal time interval [9]. Perhaps this phenomenon in the elastic case is related to the inelastic collapse. The extension of the calculation in Ref. [9] to the inelastic case is nontrivial because inelastic dynamics violates detailed balance.

We turn now to the consequence of the collapse singularity in many particle systems. Figures 4–6 show a selection of final [6] configurations in simulations with $N=1024$ disks and a solid fraction of $\nu=\frac{1}{4}$. In these three figures the solid disks are all of the particles that have been involved in the last 200 collisions of the simulation.

In Fig. 4 the coefficient of restitution is $r=0.99$ and the number of collisions is $C/N=400$. This is an example of what might be called the "kinetic regime:" the inelastic disks behave much like molecules in a gas and there is no spontaneous clustering. The continuum models described in [1] are probably valid in this case. We have compared the rms fluctuation in solid fraction [8] $\nu_{\rm rms}$ for simulations with $r=0.99$ with $\nu_{\rm rms}$ for simulations with $r=1$. The simulations with $r=0.99$ do have a slightly larger value of $\nu_{\rm rms}$ so that there is a statistically significant amount of clustering in Fig. 4 although this is not apparent to the eye.

In Fig. 5 $r=0.8$ and the number of collisions is $C/N=400$. This is an example of the "clustered regime" in which the density becomes spontaneously nonuniform but there is no finite time singularity. For instance, we have advanced simulations such as that shown in Fig. 4 until $C/N=3000$. Although the energy is monotonically decreasing

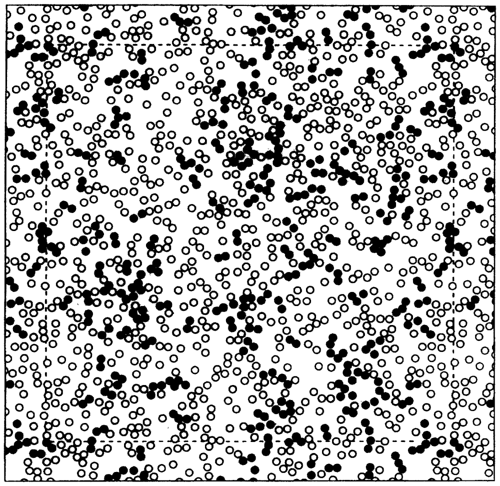

FIG. 4. The final ($C/N=400$) "kinetic regime" configuration of $N=1024$ inelastic disks with $\nu=\frac{1}{4}$ and $r=0.99$. The solid disks are all the particles that participated in the final 200 collisions of this simulation.

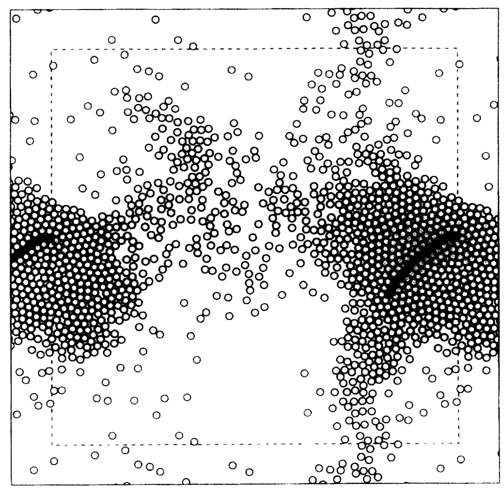

FIG. 6. The final ($C/N=68.3$) "collapsed regime" configuration of $N=1024$ inelastic disks with $\nu=\frac{1}{4}$ and $r=0.6$. The solid disks are all the particles that participated in the final 200 collisions of this simulation.

there is a statistically steady state in the sense that quantities such as $\nu_{\rm rms}$ achieve stationary values.

The transition from the kinetic regime (Fig. 4) to the clustered regime (Fig. 5) is a long wavelength instability which is described by the kinetic theories [1]: see Refs. [3] and [4]. The simulation in Fig. 4 does not form clusters because the domain is too small to contain the linearly unstable waves.

In Fig. 6 $r=0.6$ and the simulation is stopped by the separation criterion [6] when $C/N=68.3$. At this point the collision count was rising vertically as shown previously in Fig. 3 and we claim that inelastic collapse occurred: Fig. 6 is an example of the collapsed regime. The most striking change between Fig. 6 and the previous two figures is the number and configuration of the solid disks. In Fig. 6 all of the particles that have participated in the final 200 collisions of the simulation are 14 solid disks in a rough straight line. In Figs. 4 and 5 the disks involved in the most recent 200 collisions are scattered without obvious correlations throughout the domain.

There is a qualitative difference in the dynamics of this system when we decrease the coefficient of restitution from $r=0.8$ (Fig. 5) to $r=0.6$ (Fig. 6). The transition between the collapsed regime and the clustered regime occurs at some intermediate value of the coefficient of restitution which we denote by $r_*(N,\nu)$.

In Fig. 7 we summarize the results of a suite of 600 simulations all with solid fraction $\nu=\frac{1}{4}$ and $N=1024$ particles.

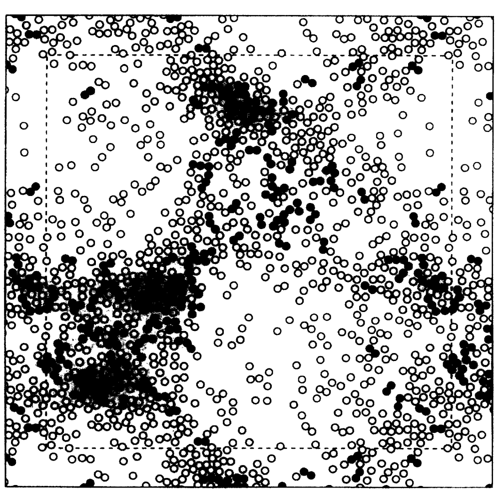

FIG. 5. The final ($C/N=400$) "clustered regime" configuration of $N=1024$ inelastic disks with $\nu=\frac{1}{4}$ and $r=0.8$. The solid disks are all the particles that participated in the final 200 collisions of this simulation.

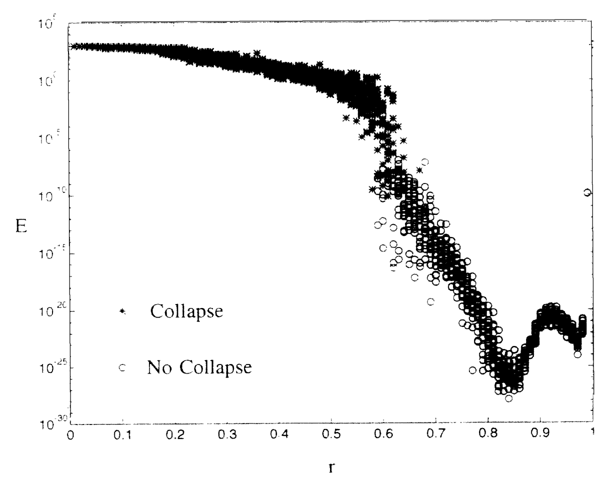

FIG. 7. The final energy in a suite of 600 simulations all with $\nu=\frac{1}{4}$ and $N=1024$. At each of 100 values of r there are six realizations. The simulations that were stopped by collapse are indicated by an asterisk while those that ran till $C/N=1500$ are indicated by an open circle.

We start at $r_1=0.01$ and proceed upwards in steps $\Delta r=0.01$ until after 99 steps the elastic limit $r_{100}=1.00$ is reached. At each value of r there are six realizations. The realizations stop if either the collision count per particle reaches $C/N=1500$ or if the separation criterion [6] with $\eta=10^{-15}$ indicates that inelastic collapse has occurred.

The ordinate of Fig. 7 shows the energy remaining in the realization when it stops. In the two limiting cases, $r=0.01$ and 1.00, all of the initial energy remains. This is obvious in the perfectly elastic case $r=1.00$. In the almost inelastic case $r=0.01$ the simulation stops in finite time so quickly that all of the initial energy is "frozen in." This explains the counterintuitive result that as r *increases* from 0.01 the final energy *decreases* up until r reaches about 0.85. We do not have an explanation for the double minima found in the region $0.80<r<1.00$.

In Fig. 7 the asterisks indicate realizations which stop in finite time because of inelastic collapse while the open circles indicate simulations that run until $C/N=1500$. The transition between the collapsed regime (*) and the clustered state (○) occurs at about $r_*(1024,\frac{1}{4})\approx 0.61$.

We do not know of any theoretical approach to calculating $r_*(N,\nu)$ in the two-dimensional case. Our simulations lead us to speculate that $r_*(N,\nu)\rightarrow 1$ as $N\rightarrow\infty$. For instance, simulations such as those in Fig. 7, but with $N=4096$, indicate that $r_*(4096,\frac{1}{4})\approx 0.77$. The single optimistic indication from our simulations is the unexpected relevance of the one-dimensional models: just as in Fig. 6 we find that with $N=4096$ the finite time singularity occurs through the formation of a nearly one-dimensional chain of disks. This phenomenon poses considerable challenges for granular kinetic theories the thrust of which has been to draw analogies between grains and molecules. Multiparticle collisions and hidden linear order have no molecular analogs. Both of these phenomena must be captured by any satisfactory theory of inelastic kinetics.

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[6] Our simulations stop if *either* (a) a predetermined number of collisions per particle C/N is reached *or* (b) immediately after one collision the next collision involves two particles whose separation is less than $\eta=10^{-15}$ (the disk diameter is one). When condition (b) is reached it means that three particles are in mutual contact, and further that one cannot accurately calculate the time to the next collision because of roundoff error. A variety of tests shows that condition (b) is not merely a computational artifact: it is also associated with a dynamic singularity such as a divergent collision frequency or a line of disks.

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