Granular collapse as a percolation transition

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Inelastic collapse is found in a two-dimensional system of inelastic hard disks confined between two walls which act as an energy source. As the coefficient of restitution is lowered, there is a transition between a state containing small collapsed clusters and a state dominated by a large collapsed cluster. The transition is analogous to that of a percolation transition. At the transition the number of clusters n_s of size s scales as $n_s \sim s^{-\tau}$ with $\tau \approx 2.7$. [S1063-651X(99)04412-8]

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There is much curent interest in developing a better understanding of the behavior of granular systems such as sand, powders, and model systems of metal and glass beads [1]. These systems can behave as a solid, liquid, or gas depending on the external conditions. However, granular systems behave very differently than molecular systems and can exhibit size segregation, avalanches, pattern formation, clustering, and collapse [2–6]. In particular, clustering and collapse have been observed not just in isolated dissipative systems, but also in driven systems [4,7,8], where energy is supplied from an external source so that the system reaches a steady state. To understand this phenomenon will likely require a number of theoretical tools.

It is thus tempting to use the traditional tools of statistical physics [9], kinetic theory, and hydrodynamics [2,10,11] to analyze the behavior of these systems. For example, a hydrodynamic description which stems from the Boltzmann equation depends on the assumption that interparticle correlations do not exist [12]. However, this work was confined to near elastic systems, and cannot explain the phenomena of inelastic collapse which can occur far from the elastic limit. Although it is possible to define a temperature proportional to the mean kinetic energy per particle, there is no thermal equilibrium equivalent to that found for molecular systems. For example, simulations and experiments have shown that granular systems do not follow a simple Maxwell-Boltzmann velocity distribution, and there is no equipartition of energy [3,7,12–15]. Hydrodynamic theories have been able to predict the length scales of clustering in granular gases [16], however, no theory has yet been able to predict the behavior of collapsed systems. In this paper we look at the inelastic collapse of a model driven granular system from the point of view of percolation theory, which describes the transition from a configuration of isolated small clusters to a configuration dominated by a single large cluster which spans the system. We will make an analogy between the percolation transition and a granular collapse transition. It is important to distinguish the phenomena of clustering from that of collapse discussed here. Clustering refers to density inhomogeneities where particles in a cluster have correlated motion. Collapse refers to the case where particles have lost essentially all their kinetic energy due to inelastic collisions. The novel aspect of our work is that the collapse of our system occurs over a wide range in the degree of inelastically, but the geometry of the collapsed particles appears to behave in a manner similar to that of a percolation transition.

To investigate the geometry of the collapsed disks in a driven system of inelastic hard disks, we use event-driven molecular-dynamics simulations [3]. The hard disks are confined to a simulation cell of size $L_x \times L_y$ with periodic boundary conditions in the x direction and hard walls at $y=0$ and $y=L_y$. The two walls are held at a fixed wall temperature T_w. All lengths are measured in units of the disk diameter. The system reaches a steady state when the energy dissipated through the collisions is compensated by energy supplied by the two walls. When a particle collides with the wall, it is ejected with a velocity whose components are distributed according to the probabilities:

$$P(v_x) = \frac{1}{\sqrt{2\pi}} e^{-v_x^2/2T_w} \quad \text{and} \quad P(v_y) = v_y e^{-v_y^2/2T_w}, \qquad (1)$$

where it is understood that v_y takes on only positive values for the bottom wall and negative values for the top wall. For elastic disks this probability distribution leads to a Maxwell-Boltzmann (MB) probability distribution for the particles near the wall. For elastic spheres it has been shown [17] that using the functional dependence of $P(v_x)$ for $P(v_y)$ [instead of using Eq. (1)] may lead to deviations from MB velocity distributions, temperatures away from the wall not equal to T_w, and unphysical inhomogeneities in density and temperature. Actual experimental systems which use vibrating walls will typically not give MB velocity distributions either. However, Grossman *et al.* [12] found that their results away from the wall were not sensitive to the details of the boundary conditions. For our purposes the only function of the wall is to input energy into the system so that the system can come to a steady state with nonzero energy. The value of using boundary conditions which give the correct MB velocity distribution for elastic disks is that we can test our program in the limit of elastic disks. In our simulations we set $T_w = 1$. The specific value of T_w merely sets the time scale in the problem. We have performed simulations with different temperatures for each wall, but the results are qualitatively similar to those found when both walls are at the same temperature.

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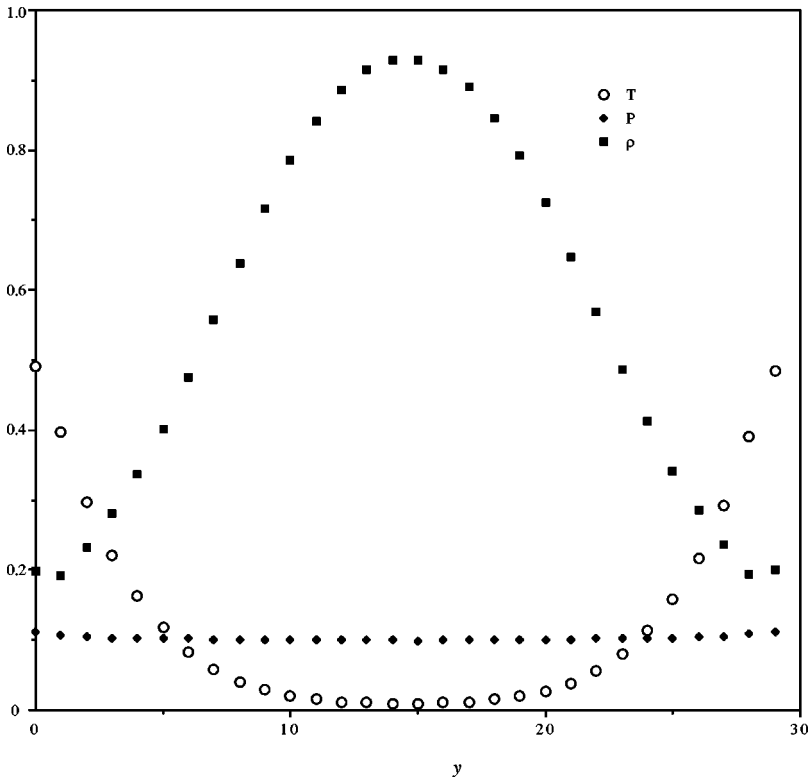


FIG. 1. The temperature T, pressure P, and density ρ as a function of position from the wall at $y=0$.

During a collision between two particles, i and j, momentum is conserved and some energy lost. We denote the component of the velocity perpendicular to the line connecting the center of the two disks by $v_{i\perp}$ and the parallel component by $v_{i\parallel}$. We denote velocities after the collision by a prime. The amount of energy lost in a collision between two disks depends on the coefficient of restitution,

$$R \equiv \frac{|v'_{i\perp} - v'_{j\perp}|}{|v_{i\perp} - v_{j\perp}|}. \tag{2}$$

The case $R=1$ corresponds to the elastic limit. By momentum conservation $v'_{i\parallel} = v_{i\parallel}$ and $v'_{j\parallel} = v_{j\parallel}$. The perpendicular velocities after the collision are given by

$$\begin{pmatrix} v'_{i\perp} \\ v'_{j\perp} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1-R & 1+R \\ 1-R & 1+R \end{pmatrix}\begin{pmatrix} v_{i\perp} \\ v_{j\perp} \end{pmatrix}. \tag{3}$$

The mechanical energy lost in the collision becomes

$$E_{\text{lost}} = -\frac{1}{4}(1-R^2)(v_{i\perp} - v_{j\perp})^2. \tag{4}$$

The initial configuration for the particles consists of a random placement of the particles in the simulation cell, with velocities distributed according to a Maxwell-Boltzmann distribution at temperature T_w. Unless otherwise specified, the number of particles is $N=500$. Typically, the system has reached a steady state after about 10^5 collisions, and the properties of the steady state are analyzed. The time used in the simulation is set such that all macroscopic quantities do not systematically change with time. The simulation is repeated for typically 100 runs to collect data.

We define a ''temperature'' T as the mean kinetic energy per particle. The behavior for the temperature, density ρ, and pressure P as a function of y is shown in Fig. 1 for a 30×30 system of 500 disks. The resolution used to make measurements is one disk diameter. The pressure can be obtained from the time-averaged impulse received by the particles during collisions. The pressure is found to be uniform throughout the system as required by mechanical stability. The density is smaller very close to the walls. This behavior occurs more strongly in relatively dense systems, and diminishes as the mean density of the system decreases. The temperature reaches a minimum and the density a maximum in the center of the system for all $R<1$. This qualitative behavior is easily explained. Particles can receive energy from the walls. As they move away from the walls, energy is dissipated in collisions. By symmetry we would expect the particles at the center to have the least energy and thus the lowest temperature. Note that the temperature of the particles whose centers are within a particle diameter of a wall is significantly less than the wall temperature $T_w=1.0$. This behavior is due to the inability of the particles to come to local thermal equilibrium. Fast moving particles, which have just picked up energy from the wall and are moving away from it, cannot thermalize with the slower particles moving toward the wall. Thus, the mean kinetic energy of the particles near the walls is an average over the higher energy particles moving away from the wall and the lower energy particles moving toward the wall. Only the temperature of the particles moving away from the wall have a temperature equal to that of the wall. If the temperatures of the two walls are different, then our simulations show a temperature minimum and density maximum that is shifted toward the lower temperature wall.

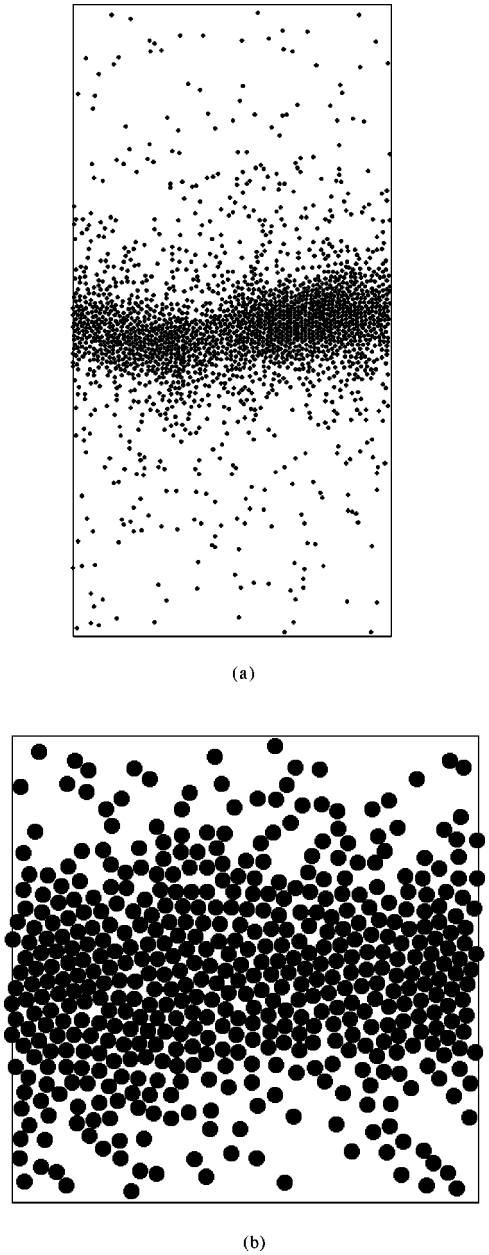
Because particles at the center have less energy, there is a tendency for these particles to pack together, and thus a den-

sity maximum occurs. We would expect this kind of behavior even in the ideal gas limit where $\rho = P/T$. Grossman *et al.* [12] developed an approximate hydrodynamic theory for their system, which worked well for values of R close to unity. We have adapted their theory to our system and found that it can reproduce the temperature minimum, but quantitative agreement is only very approximate, even at values of R near unity.

For R close to unity and a sufficiently low density of particles, the system will consist of a small number of slow moving particles N_s, defined as particles with a kinetic energy less than 0.01. The value of the kinetic energy cutoff was chosen so that the cluster labeling discussed below is insensitive to small changes in this value, and that the cutoff is low enough that there would be very few particles emerging from the wall with a kinetic energy lower than the cutoff. As R is lowered, the number of slow moving particles increases, and some of the slow moving particles begin to cluster into groups of disks in a collapsed state. This becomes evident because the mean distance moved by slow particles during a collision is of order 10^{-4} of a disk diameter. Particles in these clusters oscillate about an equilibrium position similar to molecules in a crystal. Even though energy is lost on each collision, there is energy pumped in from the surface of the collapsed clusters due to faster moving particles which are not part of the collapsed cluster. Thus, the kinetic energy of particles in the collapsed clusters does not vanish. However, these collapsed clusters do not occur for the same reason as elastic hard disk (or sphere) solidification. In the latter case hard disks can have any amount of kinetic energy, because the kinetic energy only determines the time scale of the simulation. Solidification occurs because of an imposed high density which restricts the motion of the disks. In the granular case here, the collapsed state occurs because the disks lose almost all their kinetic energy. The mean density of our simulation cell is well below the freezing density for hard disks.

Two nearby slow particles are defined to be in the same cluster if they are separated by a distance less than 1.05. This cutoff definition was chosen so that small changes in its value do not change the definition of the clusters. A continuum version of the Hoshen-Kopelman algorithm [18] is used to define the clusters. Lowering R leads to clusters of larger size, and eventually to a state with one large collapsed cluster and several very small clusters. At this point, typically the second largest cluster is less than one-fifth the size of the largest cluster. The largest cluster has a stable hexagonal crystal structure with only its surface changing with time during the time scale of our simulations. Thus, the particles can be divided into two groups: those that are part of collapsed solidlike clusters of particles which are moving very slowly, and a dilute collection of uncorrelated particles which are moving quickly and thus constitute a granular gas. Figure 2 shows snapshots of two systems which contain a large solidlike cluster surrounded by smaller clusters and isolated disks. These snapshots are typical of what is seen near the transition. As R is lowered the solidlike largest cluster grows and its hexagonal crystal structure contains fewer defects.

The above scenario is analogous to that found in standard percolation theory, where cluster properties are calculated as



(a)

(b)

FIG. 2. Snapshots of two systems which contain a solidlike cluster. The parameters are (a) number of particles $N=2000$, linear dimensions $L_x=80$, $L_y=160$, and coefficient of restitution $R=0.89$; (b) $N=500$, $L_x=L_y=30$, $R=0.85$.

a function of a parameter p which is the fraction of occupied sites (for a lattice model) or a volume fraction of the space covered by the objects of interest. At $p=p_c$, one large cluster forms which spans the entire system. The percolation threshold becomes more sharply defined as the size of the system increases. In the infinite size limit, the connectedness length ξ, which is a measure of the linear dimension of the nonspanning clusters, diverges as $\xi \sim |p-p_c|^{-\nu}$. The mean size of the nonspanning clusters χ diverges as $\chi \sim |p-p_c|^{-\gamma}$. The fraction of the occupied space which is part of the spanning cluster P_{span} vanishes as $(p-p_c)^{\beta}$, where β is another critical exponent. In addition at p_c the number of clusters of size s per lattice site n_s scales as $n_s \sim s^{-\tau}$. Scaling theory leads to the relations $2\beta+\gamma=\nu d$ and $\tau=2+\beta/(\beta$

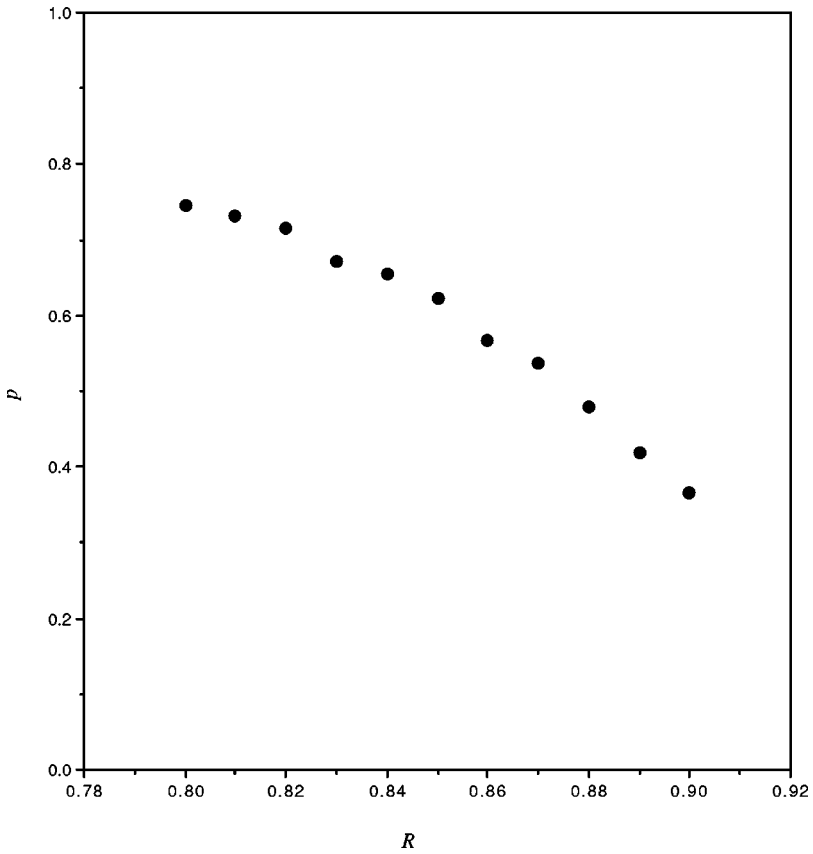


FIG. 3. The fraction of slow particles p as a function of R with $N=500$, $L_x=L_y=30$, averaged over 100 runs.

$+\gamma$) [19]. The exponents ν, γ, β, and τ depend only on the dimensionality d of space.

Percolation theory has been very useful for describing a large variety of randomly disordered systems. The theory provides a guide for determining which quantities show power-law behavior near a transition. In addition the theory makes many universal predictions which are independent of the details of how the disorder is created. For these reasons, we believe it is useful to describe granular collapse in our system with percolation theory as a guide.

To make the analogy with percolation theory, we define $p=N_s/N$. At $p=p_c$ we expect to see collapsed clusters of all sizes in the limit as $N\rightarrow\infty$. In analogy to percolation theory we define a spanning cluster as a cluster which spans the simulation cell in the x direction. Explicit formulas for calculating the percolation quantities are as follows. The connectedness length is given by

$$\xi^2=\frac{1}{2}\frac{\sum_{k=1}^{N_c}\sum_{i}\sum_{j} r_{i,j,k}^2}{\sum_{k=1}^{N_c} s_k^2}, \tag{5}$$

where N_c is the number of collapsed clusters not including the spanning cluster, $r_{i,j,k}$ is the distance between disk i and disk j in cluster k, and s_k is the number of disks in the kth cluster. The mean cluster size is

$$\chi=\frac{\sum_{k=1}^{N_c} s_k^2}{\sum_{k=1}^{N_c} s_k}. \tag{6}$$

Another useful quantity is the fraction of runs which contain a spanning cluster which we denote by f. We define P_{span} as the number of particles in the spanning cluster divided by N_s.

Figure 3 shows how p depends on R for a 30×30 simulation cell with $N=500$ particles. Because the dependence is smooth over the entire range of R, we expect any power-law behavior to be the same as a function of R or p. Figure 4 shows the results for the quantities f, P_{span}, ξ, and χ. These results are qualitatively similar to those found in typical continuum percolation systems. Our system sizes are much too small to be able to extract reliable critical exponents or a precise value of p_c. However, if we define p_c as the value of p where $f=1/2$ and make crude estimates for the critical exponents, we find $\nu\approx1$, $\gamma\approx1.5$, and $\beta\approx0.5$. The estimates for ν and γ are approximately the same above and below the transition, a result expected from percolation theory. Our values lead to $2\beta+\gamma=2.5$ and $2\nu=2$. Because our estimates are very crude this scaling relation cannot be ruled out. For comparison the values found in standard two-dimensional (2D) percolation are $\nu=4/3$, $\gamma=43/18$, and $\beta=5/36$. Much better statistics with a larger number of disks would be needed to estimate the percolation exponents reliably and determine if scaling exists.

Near p_c, the power-law dependence of the cluster size distribution is robust and always shows a critical exponent of $\tau\approx2.7$ for several different values of N and cell size, including asymmetric simulation cells such as a 20×160 cell. Figure 5 shows typical log-log plots of n_s versus s. For $N=1000$ we have a sufficient number of runs and number of disks to obtain statistics on clusters up to size $s=30$. For the other systems the plots show data for clusters up to size s

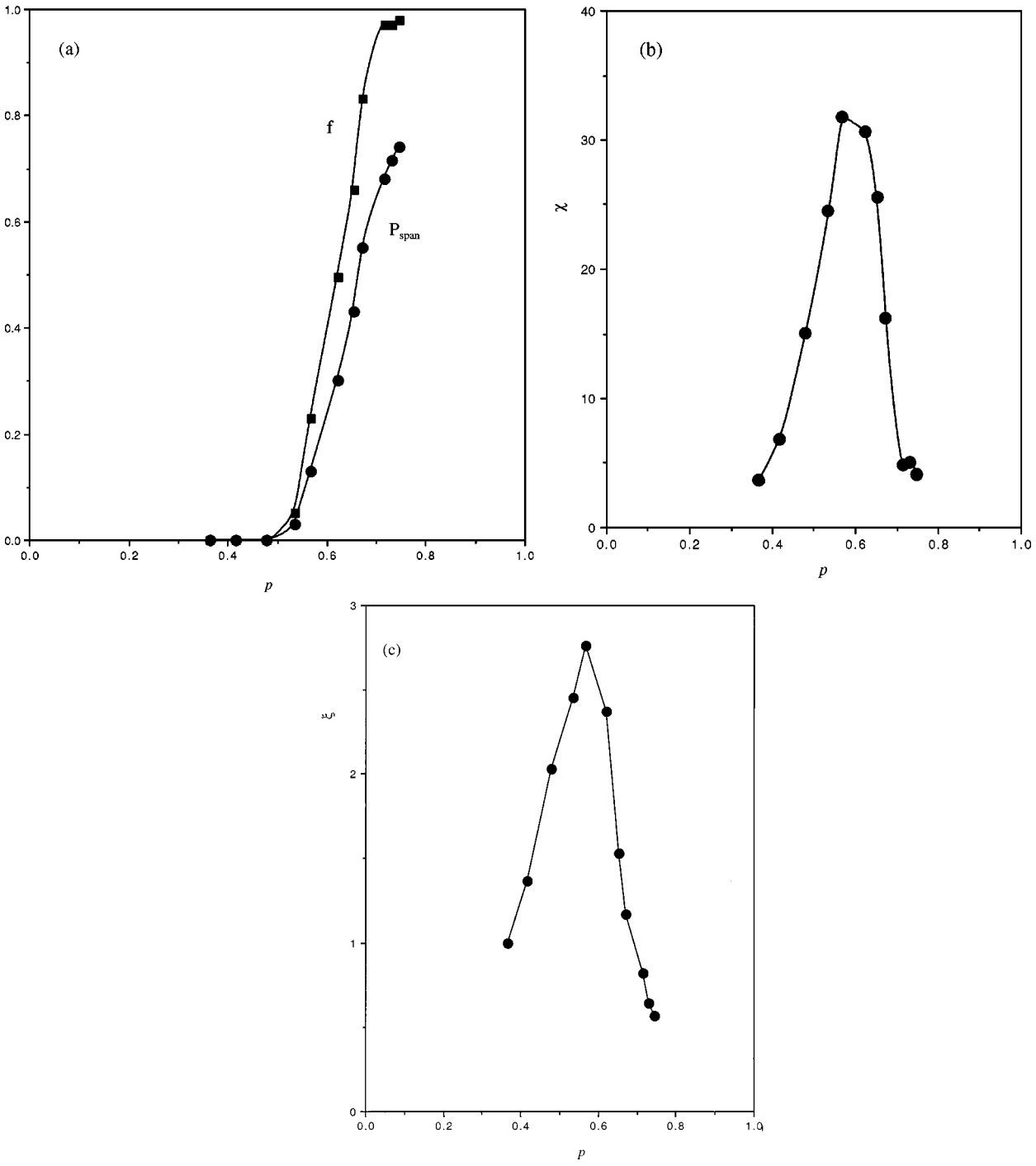


FIG. 4. Percolation properties as a function of the fraction of slow particles p. (a) Plot of f, the fraction of runs which contain a spanning cluster, and P_{span}, the fraction of slow particles in the spanning collapsed cluster; (b) the mean cluster size χ, and (c) the connectedness length ξ in units of the disk diameter. Properties computed from the same system as in Fig. 3. The statistical uncertainties of χ and ξ are approximately 10%. The curves are only guides to the eye.

$=10$. This estimate for τ is much different than that found in standard 2D percolation where $\tau=187/91\approx 2.06$. If our result for τ is approximately correct, then it is very difficult to see how the scaling result $\tau=2+\beta/(\beta+\gamma)$ could be valid. One possibility is that the relationship between cluster numbers and the other percolation quantities is not the same as that found in standard percolation theory. This could be because in our case there is a systematic variation in density from one wall to the other in the y direction, and for L_y large enough our results are independent of L_y once a steady state has been reached. Thus, no cluster properties are normalized by the linear dimensions of the system. On the other hand, standard percolation systems do not have this systematic inhomogeneity, and cluster numbers are normalized by the linear dimensions of the system. Another possibility is that our estimates for the critical exponents are too crude.

Many of the features we observe are similar to those found in percolation theory. The connectedness length and mean cluster size grow very quickly with small changes in the coefficient of restitution near the transition in analogy to

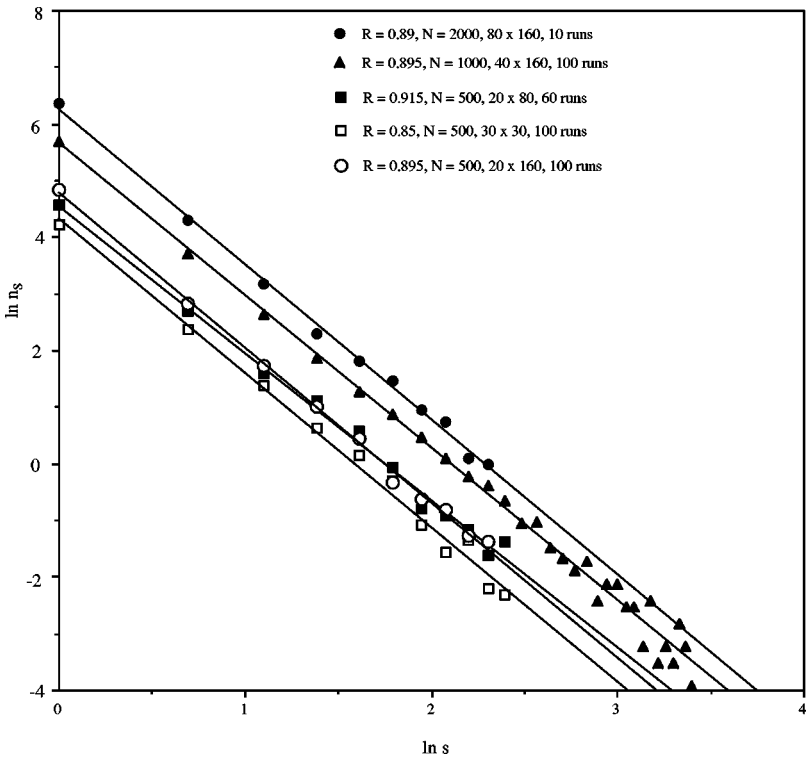


FIG. 5. Log-log plot of the mean number of clusters n_s of size s versus s for five different systems. The lines are least-squares fits for each system. The average of the slopes is 2.7.

how these quantities grow quickly as a function of an occupation factor p in percolation systems. There are large variations from run to run in percolation quantities near the transition suggestive of the the critical fluctuations one finds near a standard percolation transition or any second-order phase transition. These critical fluctuations are due to the presense of structures of all length scales. Our robust power-law behavior for the cluster size distribution provides further evidence for a true phase transition in the limit $N \rightarrow \infty$.

In summary, we have described the inelastic collapse of a model system of granular material in terms of percolation type quantities. We have found that the number of clusters of size s behaves as a power law, and that other quantities behave in a way similar to analogous quantities in percolation theory. Much larger systems are needed to find quantitatively precise values of the exponents analogous to critical percolation exponents. These results suggest that the geometry of collapsed clusters may be an important universal feature of collapse in driven granular systems.

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