Simulations of granular gravitational collapse

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A freely cooling granular gas in a gravitational field undergoes a collapse to a multicontact state in a finite time. Previous theoretical [D. Volkson et al., Phys. Rev. E 73, 061305 (2006)] and experimental work [R. Son et al., Phys. Rev. E 78, 041302 (2008)] have obtained contradictory results about the rate of energy loss before the gravitational collapse. Here we use a molecular dynamics simulation in an attempt to recreate the experimental and theoretical results to resolve the discrepancy. We are able to nearly match the experimental results, and find that to reproduce the power law predicted in the theory we need a nearly elastic system with a constant coefficient of restitution greater than 0.993. For the more realistic velocity-dependent coefficient of restitution, there does not appear to be a power-law decay and the transition from granular gas to granular solid is smooth, making it difficult to define a time of collapse.

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I. INTRODUCTION

When a granular gas evolves freely in gravity without additional energy input, inelastic collisions cool the gas and freeze it into a granular solid in a finite time [1,2]. The role gravity plays in the transition from collision-dominated dynamics to multiple contact dynamics is well researched in some density regimes, as in granular impact craters [3,4] or the transient flow after failure of a granular step [5,6]. Yet the role gravity plays in the transition from collision-dominated kinetic theory. We have selected five simulations of different pile depths (short and tall), coefficient of restitution (constant 0.55 and 0.95, the parameters would be $\epsilon = 0.056$ and $\Lambda = 2.79$, of similar magnitude to the theory. The system was fluidized by vibrating the chamber, and decay was initiated by ceasing the vibrational energy input. Photographs were taken at high time and space resolution, particles were tracked by position and velocity, and statistics were collected from the resulting tracks of many similar decays; Fig. 1(b) shows the granular temperature as a function of height and time from the experiment in Ref. [2].

Our goal in this paper is to explore the reasons for the divergence between the theoretical result and experimental observation by using a molecular dynamics model. With it, we can observe different decay behaviors as system parameters are varied between the experimental conditions and the limits used in the theory. We have selected five simulations of different pile depths (short and tall), coefficient of restitution (constant and velocity dependent), and frictional interactions (with and without tangential friction) to highlight these differences and clarify the range of applicability of the previous results.

II. SIMULATION

To study the decay, we adapted a three-dimensional molecular dynamics simulation developed by Shattuck that integrates Newton’s law for each soft sphere using a verlet method. A two-dimensional version of this code was used by the authors

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of Ref. [12]. We modeled a chamber with approximately the same dimensions as the setup of Son et al. [2]. We allowed for fully three-dimensional motion and rotation caused by friction tangential to the surface of the particles to replicate the quasi-two-dimensional (2D) nature of the experiment. For simplicity, the walls were all assumed to have the same properties as the particles. To collect statistics from unique decays, we randomized the initial velocities for particles in positions saved from a previously fluidized state and simulated chamber driving to ensure the system reached a steady state before starting the decay. The particular instant we chose to stop the driving was consistent with the experimental design of the authors of Ref. [2] and should not appreciably affect the dynamics during decay because the driving period is very short compared to the decay time. Data collection was restricted to particles at least one diameter from the side walls to avoid boundary effects.

We tried two different force laws that have been widely used in the literature [13,14] to model the interactions between particles. The first model is a truncated Hooke’s force with linear dissipation, called the linear-spring-dashpot (henceforth, Hooke’s) force, and is given by

\[
F = \begin{cases} 
0 & \text{if } \xi > 0, \\
-k\xi - \gamma\dot{\xi} & \text{if } \xi < 0, 
\end{cases}
\] (2)

with \(\xi\) the overlap of one particle on another, \(\dot{\xi}\) its time derivative, \(k\) a coefficient of elasticity, and \(\gamma\) a coefficient of energy dissipation. This force results in a constant coefficient of restitution [15]. Maintaining particle stiffness at energy dissipation. This force results in a constant coefficient with \(\xi > 0\) if \(\xi < 0\), (2)

The benefit of this model of particle interaction is its velocity-dependent coefficient of restitution [18], consistent with empirical observations that the coefficient of restitution drops off with impact velocity \(v\) like \(v^{1/3}\) [16] and similar theoretical predictions [19]. With \(k = 3.42 \times 10^9 \text{ N/m}^{3/2}\) and \(\gamma = 2.54 \times 10^4 \text{ kg/m/s}^{1/2}\), we found the coefficient of restitution was fit very well by the function

\[
r = 1 - 0.81v^{1/5},
\] (4)

and had a statistical mean \(r = 0.94 \pm 0.012\), which matched the particles used by the authors of Ref. [2] and allowed immediate comparison to that experiment. This fit was performed on data from a sample of 50 simulated head-on collisions with random impact velocities between 0 and 0.9 m/s, which covers the range of experimental velocities during the steady state.

Figure 1 shows the granular temperature as a function of time from (a) our simulation and (b) the experiment in Ref. [2]. The figure shows the last two periods of drive and the subsequent collapse. The data from the simulation were compiled from 320 independent decays initialized as previously described. To match the experiments we used the Hertz force with tangential friction (coefficient of kinetic friction, \(\mu = 0.3\)). The temperature field for the simulation is qualitatively very similar to the experiment. During the fluidized state, the gas has shockwaves extending about halfway through the system with a section of relatively uniformly heated gas [20]. A collapse shock is clear around 0.1 s, during which the energy in the mean flow is converted to fluctuating thermal energy through interaction with the bottom boundary [1,2]. This shock is followed by the final stage of collapse when the particles partially crystallize and settle into their final multiple-contact state.

There are a few important differences to note between the simulation and experiment. The simulation has slightly higher granular temperature all throughout the decay, which results in more particles striking the top of the chamber and a more intense collapse shock. The effects of the collisions with the top plate are small, however, because of the low density at the top of the chamber. The simulation has a slightly more intense collapse shock which shifts the beginning of the final collapse. Some of these differences are likely the result of aspects of the experiments that the simulations did not match, including air in the chamber, different interactions with aluminum and glass walls, and maybe electrostatic effects. However, part of the differences are simply that simulation parameters have not been completely matched to the experiments since many parameters were not measured experimentally and it is computationally expensive to tune
them by trial and error. Beyond these small differences, the resulting collapse dynamics in the simulation are a good match to the experiment, from the shape of the collapse shock to the time for total decay.

III. RESULTS

A. From experiment to theoretical limit

Figure 2(a) shows the spatially averaged granular temperature associated with each time step from Fig. 1(a). Vibrational energy input is ceased at time $t = 0$ and the particles begin their gravitational collapse. The heating effects of the collapse shock, seen here at approximately 0.075 s into the decay, are immediately apparent on this plot as a local maximum in the averaged granular temperature. Past this time, the system enters the final stages of collapse, where inelastic collisions dissipate the remaining granular temperature and the system comes to rest.

To compare different power-law fits, Fig. 2(b) shows the average granular temperature on a semilogarithmic scale along with two nonlinear least squares fits of Eq. (1). One fit uses all three free parameters, $T_0$, $t_c$, and $n$, while the other fit fixes $n = 2$. They are both fit over the same time interval from 0.1 to 0.21 s. Neither of these fits is a particularly good match to the data, but $n = 2$ is a much poorer fit than the one which estimates $n = 9.2$.

These nonlinear fits to a power law with a time offset as a fit parameter show the sensitivity of the best-fit estimates to the initial guesses and data ranges used. So we will report ranges of the fitted parameters and remain open to the possibility that a power law may not accurately describe each system. Occasionally, a data set would result in a set of best-fit parameters very much an outlier from the rest. In these cases, that particular parameter combination was evaluated for the quality of the fit and, if necessary, was not counted for use in the reported range. On several of the data sets, we used multiple fitting routines to verify the results and to be sure that when fits were inadequate, it was because of the imposed functional form and not the fitting procedures.

For the data in Fig. 2, the power-law fit is not very good. We obtained fits with power-law exponents ranging from $n = 5$ to $n = 9.5$, which corroborates the high values found by the authors of Ref. [2].

Having confirmed that we see gravitational collapse dynamics that are very similar to the experiments in Son et al. [2] when we try to match their parameters, we modified our simulation to move closer to the parameters used in Volfson et al. [1]. We confined the particles to a 2D plane and removed tangential friction. We also doubled the number of layers of particles for $\epsilon = 0.029$. We still use the Hertz interparticle force. Figure 3 shows the effects of these changes. Similar to the decay in Fig. 2, this decay diverges considerably from a power law. If we try to fit a power law we get exponents ranging from 3.5 and 7.1 for different subsets of the range. Though the fits estimate a collapse time within $t_c \in [0.49 s, 0.64 s]$, there is considerable energy beyond these times. We conclude that friction, the quasi-2D chamber, and the small number of layers are not the reason that the experiments deviate from the theoretical predictions.

![Figure 2](image-url)

**FIG. 2.** (Color online) (a) The decay of granular temperature for the simulation results shown in Fig. 1. $N_p = 285$, $\epsilon = 0.056$, and 1.73 $< \Lambda < 3.41$. This range of $\Lambda$ reflects the fact that the coefficient of restitution is not constant and we give the value for the minimum and maximum coefficients of restitution. (b) The data are shown on a semilog scale with two associated best fits to Eq. (1) over the same time interval. One fit forces $n = 2$ (blue, long dashed line) and fits $T_0$ and $t_c$ and the other (red, wide dashed line) fits all three parameters to find $n = 9.2$. We see that power-law behavior is unlikely.

![Figure 3](image-url)

**FIG. 3.** (Color online) Granular temperature decay for a system with no tangential friction, confined to two dimensions, and containing more particles $N_p = 570$. Hertz force with $r \approx 0.94$, $\epsilon = 0.029$, and 3.43 $< \Lambda < 6.76$. Power-law fits are shown and, like in Fig. 2, the best-fit power law has $n$ much greater than 2 and is not a very good fit.
dependence with estimates for the collapse time. We see that the potential power laws without assuming a collapse time. We

1. For a visual guide to evaluate the specifics of power-law behavior, Fig. 4(b) displays the data on a linear scale, to the

1/n power. This allows us to visually distinguish between potential power laws without assuming a collapse time. We

see that the n = 2 line has upward curvature, whereas the

n = 5 line begins to look convex. Alternatively, n = 3 and n = 4 look relatively straight, thus verifying the estimated range between n = 3.2 and n = 4.6. Although a power law seems to be more accurate than for the previous data sets, the power is considerably higher than the predicted n = 2.

Figure 5 shows the decay from another set of simulations with a deeper pile of particles interacting through Hooke’s force, here for a constant coefficient of restitution of r = 0.96. As a result of the deeper pile and rapid energy loss in the early stage, a well-defined collapse shock is now observable (around t = 0.18 s), the only simulation in which this dynamical feature was observed for a constant coefficient of restitution. The set of estimated values for n is somewhat similar to the values for the shallower simulations with Hooke’s force (Fig. 4), spanning values between n = 3.8 and n = 4.2. This implies that there is little sensitivity to r in the range considered.

To obtain results close to the prediction of the authors of Ref. [1] we find that we need to use the constant coefficient of restitution and very small inelasticity. Figure 6 shows decay statistics collected from a deep system with r = 0.993. Several features immediately set it apart from the dynamics observed experimentally. The most notable difference is the complete lack of collapse shock. Additionally, the duration of this decay is an order of magnitude higher, with t_c ∈ [3.6 s, 3.9 s]. Both of these observations are consistent with the expected dynamics of a system with very low energy loss rate. Figure 6 indicates a power-law time dependence is a much better fit to these
data throughout practically the entire decay. The nonlinear fits result in exponents between \( n = 2.3 \) and \( n = 3.5 \). In Fig. 6(b), the best fit seems to be between \( n = 2.5 \) and \( n = 3 \), quite a bit closer to the theoretical prediction than observed by the authors of Ref. [2].

Table I summarizes the power-law exponents collected from the various runs described above. Note the trend from top left to bottom right of decreasing estimates for \( n \) in the different runs. As we progress from the experimental setting to more and more ideal settings of a constant, high coefficient of restitution, we see a trend in the direction of the \( n = 2 \) prediction. A clear difference exists between systems with the Hertz force and the Hooke’s force. Friction and pile depth certainly affect the dynamics and change the rate of decay, but the effect of the assumptions for the coefficient of restitution appears to be much more dominant in governing the form of the decay law.

**TABLE I.** The ranges of the estimated power-law exponent, \( n \), in \( T \propto (t-t_c)^n \) [Eq. (1)], for each of the data sets presented.

<table>
<thead>
<tr>
<th>( N_p )</th>
<th>Hertz force ( n )</th>
<th>Hooke’s force ( n )</th>
<th>Hooke’s force ( r )</th>
</tr>
</thead>
<tbody>
<tr>
<td>285</td>
<td>5–9.5 (with friction)</td>
<td>3.2–4.6</td>
<td>0.96</td>
</tr>
<tr>
<td>570</td>
<td>3.5–7.1 (no friction)</td>
<td>3.8–4.2</td>
<td>0.993</td>
</tr>
</tbody>
</table>

FIG. 6. (Color online) Granular temperature decay for \( N_p = 570 \) and \( r = 0.993 \), or \( \epsilon = 0.029 \) and \( \Lambda = 2.04 \). (a) The data on a semilog scale with two best fits over the same subset of data. Note that there is no collapse shock. (b) The late states of the decay to the 1/n power. A power-law exponent between \( n = 2.5 \) and \( n = 3 \) is a good fit, much closer to the predicted \( n = 2 \) than the decay of Fig. 2.

At the end of Fig. 6(a), the decay appears to enter a new regime of slower energy loss. This effect was observable in all of the runs of the simulation, at late times when the particles are in constant contact. The rate of energy loss in this regime depended on particle stiffness, and the transition was different between the Hooke and Hertz forces. This is most clearly seen in a one-dimensional (1D) system with a small number of particles.

**B. Very late stage of collapse**

Figure 7(a) shows the results of 1D simulations with ten particles of different stiffnesses interacting with Hooke’s force. The column of particles was fluidized by an oscillating base which was then halted, allowing the particles to collapse. The trend after the initial gravitational collapse dynamics is an exponential decay that depends on the particle stiffness. It appears that this second regime of decay begins once the particles enter a state of permanent multiple contacts. Here the particle motion consists of the phonon modes of a material with
dissipative harmonic interactions, and exponential decay is expected. The absolutely final stages of hard-sphere dynamics are inaccessible as a result of the vibrational modes in the soft-sphere approximation and computer round-off.

Figure 7(b) shows the kinetic energy for both Hooke’s and Hertz forces with ten particles in 1D and with the same parameters used in the simulation runs of Figs. 2 and 4. Here we see clearly that the Hertz force data deviates from a power law much more than the Hooke’s force data. The Hertz case exhibits positive curvature as it enters the stage of permanent multiple contacts and has a smooth transition between collisional dynamics and multiple contact dynamics. As the system cools, the energy loss rate decreases via the velocity dependence of the coefficient of restitution [19]. Thus we observe that the time of collapse when the system transitions to the elastic vibrational modes is much less well defined. A velocity-dependent coefficient of restitution produces very different dynamics than a constant coefficient of restitution near the collapse from a granular gas to a granular solid.

IV. CONCLUSION

The problem of inelastic collapse of a granular gas in gravity is a prototypical simple system with quite complex dynamics. Previous work on this problem had produced a theoretical description of the approach to the static state [1], but experiments did not agree with the theory [2]. Our simulations here confirm that the experiments provide reliable measurements of the dynamics of this system. We are able to match the phenomenology that was observed in the experiments and we find good quantitative agreement with the functional form of the energy loss just before collapse. We find that the disagreement with the theory is not the result of nonideal experimental conditions such as the quasi-2D chamber, small pile depth, or even the existence of tangential friction. Rather, matching the existing theoretical prediction in our simulations seems to require the use of a velocity-independent coefficient of restitution in the limit of very small inelasticity.

This system of gravitational collapse of a granular gas appears to be an excellent candidate for a standard test case for theories of dense granular gasses. It has simple behavior in the nearly elastic limit that is currently understood theoretically. However, existing experiments and most applied situations involve gravitational collapse at parameters that are not adequately described by existing theories.

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