Dynamics of Freely Cooling Granular Gases

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We study dynamics of freely cooling granular gases in two-dimensions using large-scale molecular dynamics simulations. We find that for dilute systems the typical kinetic energy decays algebraically with time, $E(t) \sim t^{-1}$, in the long time limit. Asymptotically, velocity statistics are characterized by a universal Gaussian distribution, in contrast with the exponential high-energy tails characterizing the early homogeneous regime. We show that in the late clustering regime particles move coherently as typical local velocity fluctuations, Δv, are small compared with the typical velocity, $\Delta v/v \sim t^{-1/4}$. Furthermore, locally averaged shear modes dominate over acoustic modes. The small thermal velocity fluctuations suggest that the system can be heuristically described by Burgers-like equations.

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Freely evolving granular media, i.e., ensembles of hard sphere particles undergoing dissipative inelastic collisions, exhibit interesting collective phenomena including clustering, vortices, shocks, and multiple dynamical regimes. This dissipative nonequilibrium gas system can be described by kinetic theory in the early homogeneous phase where density fluctuations and velocity correlations are relatively small. However, quantitative characteristics of the late clustering regime such as the typical length and velocity scales, particle velocity distributions, as well the corresponding continuum theory remain open questions [1–19].

Recent molecular dynamics simulations in one-dimension have shown that the asymptotic energy decay is universal and that clustering corresponds to the formation of shocks in the inviscid Burgers equation [12]. In this paper we study long time asymptotic dynamics of freely evolving granular gases in two dimensions using Molecular Dynamics (MD) simulations. Treating the particles as identical, totally undeformable hard disks, we developed an efficient event-driven algorithm [20–22] that allows us to probe the system well into the clustering regime. Our main result is that the asymptotic dynamics of dilute granular gases is universal as it is independent of the degree of dissipation.

In the simulations, $N = 10^6$ identical disks of radius $R = 0.15$ and mass $m = 1$ are placed in a two-dimensional system of linear dimension $L = 10^3$ with periodic boundary conditions. The particle concentration, $c = 1$, so the mass density (or volume fraction) is $\alpha = c\pi R^2 = 0.0707$. Initially, particles are distributed randomly in space and their velocities are drawn from a Gaussian distribution with zero mean and unit variance. To ensure random initial conditions, the system is first evolved under elastic collisions only, with each particle undergoing 10^2 collisions on average. Then, time is reset to zero and each particle experiences up to an average of 4×10^4 inelastic collisions. In such a collision the particle velocity, $\mathbf{v}$, changes according to

$$\mathbf{v} \to \mathbf{v} - \frac{1}{2}(1+r)(\mathbf{g}\cdot\mathbf{n})\,\mathbf{n}, \tag{1}$$

with $\mathbf{g} = \mathbf{v} - \mathbf{v}'$ the relative velocity of the colliding particles and $\mathbf{n}$ a unit vector connecting the centers of the two particles. In each collision, the normal component of the relative velocity is reduced by the restitution coefficient, $0 \le r \le 1$, and the energy dissipation equals $\frac{1}{2}(1-r^2)(\mathbf{g}\cdot\mathbf{n})^2$. In the following, time is quoted in units of $t_0 = \frac{3}{20cR}\sqrt{m/E_0}$ which is proportional to the initial mean free time, where E_0 is the average particle energy initially.

Inelastic collapse, the formation of a cluster via an infinite series of collisions occurring in a finite time, poses a difficulty for numerical simulations [4]. To properly resolve such finite time singularities, we take collisions to be perfectly elastic ($r = 1$) when the relative velocity falls below a pre-specified threshold $\mathbf{g}\cdot\mathbf{n} < \delta$. This scheme, which mimics actual granular particles where $r \to 1$ for sufficiently small relative velocities, can be applied as long as the cutoff velocity δ is much smaller than the root mean square (rms) velocity, $v_{\rm rms} \equiv \langle v^2\rangle^{1/2}$ [12,23]. In our simulations, $v_{\rm rms} > 10^{-3}$, and $\delta = 10^{-5}$.

Given the initial conditions, the collision sequence is deterministic, and the system evolves freely (velocities are not controlled). In the absence of energy input, the system "cools" infinitely. The average particle energy, $E(t) = \frac{1}{2}\langle v^2\rangle$, as a function of time is shown in Fig. 1. First, we confirmed that for sufficiently small times, when the spatial distribution of particles remains roughly uniform, the energy decay follows Haff's cooling law [1]

$$E(t) = E_0\,(1 + t/t_*)^{-2}\,. \tag{2}$$

Here, $(t_0/t_*)^{-1} = 3\sqrt{\pi}(1-r^2)g(2R)/20$, where $g(r)$ is the pair correlation function [10,11].

However, this cooling law eventually breaks down due to the formation of dense clusters [3,7,9,11–13,15]. The deviation from this law occurs at a time scale that ultimately diverges when collisions become elastic. Interestingly, our simulations show that a universal decay law

$$E(t) \simeq A(r)t^{-1}, \quad (3)$$

holds beyond this time scale. This implies that the typical velocity decays with time according to $v \sim t^{-1/2}$. The typical length scale explored by a particle, $\mathcal{L}(t) \sim \int_0^t dt' v(t') \sim t^{1/2}$, remains small compared with the system size, $\mathcal{L} \ll L$, and thus, finite size effects were negligible throughout the simulations. The inset to Fig. 1 shows that the energy decay law is independent of the cutoff velocity as long as $\delta \leq 10^{-4}$ (we also verified that numerical errors were irrelevant).

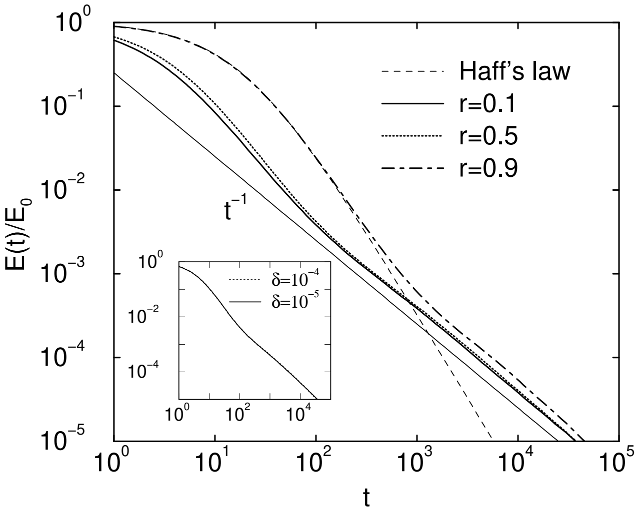

FIG. 1. The average particle energy $E(t)$ as a function of time t for three different restitution coefficients, $r = 0.1$, 0.5, and 0.9. A line of slope -1 is shown for reference. The inset shows $E(t)$ as a function of t for $r = 0.1$ and different cutoffs $\delta = 10^{-4}$, 10^{-5}. Each line represents an average over four independent realizations.

Overall, this behavior is consistent with the r-independent energy decay law, $E \sim t^{-2/3}$, found in one-dimension [12], although the exponent differs from the 1D value of 2/3. This asymptotic law (3) has not been observed in previous numerical studies primarily due to insufficient temporal range [3,7,9,11,13,15]. For example, power-law behavior was previously suggested by deformable sphere molecular dynamics simulations in two- and three-dimensions [13]. However, the value of the scaling exponent depended on parameters such as the system size and the restitution coefficient.

The simulations show that as the volume fraction α was reduced, the dependence of the prefactor $A(r)$ on the restitution coefficient r became weaker and weaker, suggesting completely universal behavior in the dilute limit, $\alpha \to 0$. Further numerical studies with smaller volume fractions are needed to fully resolve this issue. If indeed the prefactor A is independent of the restitution coefficient r, this implies a certain behavior of t_c, the time scale marking the transition from the homogeneous to the clustering regime. Matching the two asymptotic behaviors $E(t) \sim [(1-r)t]^{-2}$ for $t \ll t_c$ with $E(t) \sim t^{-1}$ for $t \gg t_c$ shows that this crossover time scale diverges according to $t_c \sim (1-r)^{-2}$ in the quasi-elastic limit, $r \to 1$.

Next, we examined whether the entire velocity distribution, not merely the typical velocity scale is independent of the restitution coefficient. We studied $P(v,t)$, the probability distribution function of the velocity magnitude $v \equiv |\mathbf{v}|$ at time t. Figure 2 clearly shows that a universal scaling function underlies the velocity distribution when $t \gg t_c(r)$

$$P(v,t) \sim \frac{1}{v_{\rm rms}^2}\Phi(z), \qquad z = \frac{v}{v_{\rm rms}}. \quad (4)$$

This provides evidence that the asymptotic dynamics are universal.

The simulations suggest that the corresponding scaling function is Gaussian, $\Phi(z) = \pi^{-1}\exp(-z^2)$, (see Fig. 2). We therefore studied the kurtosis, particularly, the quantity $\kappa = \langle v^4\rangle/\langle v^2\rangle^2 - 2$. Initially, $\kappa = 0$, the expected value for a Gaussian distribution in two-dimensions. In the intermediate regime, κ is distinctly nonzero and strongly depends on the value of the restitution coefficient. However, in the asymptotic regime ($t \gg t_c$), κ does not depend on restitution coefficient and is very close to zero ($|\kappa| < 0.1$), a manifestation of the universal velocity statistics. Given this universality, we present data for a representative value of $r = 0.1$ in the rest of this paper.

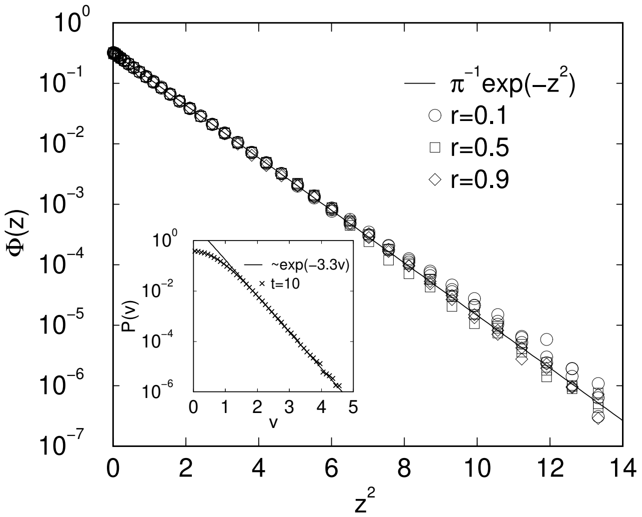

FIG. 2. The scaling velocity distribution $\Phi(z)$ versus the square of scaling variable $z = v/v_{\rm rms}$. The data corresponds to three different restitution coefficients $r = 0.1$, 0.5, and 0.9, at three different times, $t = 5 \times 10^2$ (excluding $r = 0.9$), 2×10^3, 2×10^4, all in the clustering regime. These eight distributions follow a universal scaling function, a Gaussian distribution. The inset shows the exponential high-energy tail of $P(v)$ at $t = 10$ for $r = 0.1$, where the velocity was rescaled by the rms velocity.

For completeness, we mention that in the intermediate homogeneous regime, the distribution has an exponential high-energy tail, in agreement with kinetic theory studies [3,8,16–19]. The measured slope of 3.3 is consistent with Direct Simulation Monte Carlo (DSMC) [17] and MD simulations [19] (see the inset in Fig. 2).

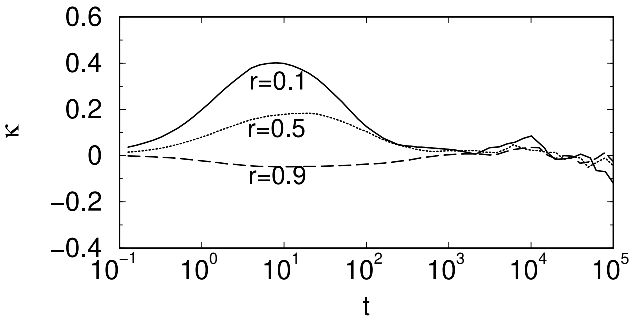

FIG. 3. The adjusted kurtosis κ as a function of time for three restitution coefficients $r = 0.1, 0.5$, and 0.9.

Both the Gaussian and the exponential extremal velocity statistics are consistent with the following heuristic argument. The large-velocity tails are dominated by the fastest particles ($v \approx 1$) initially present in the system, still moving with their initial velocity at time t. These particles managed to avoid any collisions with other particles. The "survival" probability, $S(v,t)$, for such particles decays exponentially with the volume they sweep till time t, $S(v = 1,t) \propto \exp(-\text{const.} \times t)$. Assuming a stretched exponential large-velocity tail for the scaling function $\Phi(z) \sim \exp(-\text{const.} \times |z|^\gamma)$ as $z \to \infty$ and the typical velocity decay $v \sim t^{-\beta}$ as $t \to \infty$, and then matching the dominant behavior of the fastest particles $P(1,t) = P(1,0)S(1,t) \propto \exp(-\text{const.} \times t)$ with the expected scaling behavior $P(1,t) \propto \Phi\left(t^\beta\right) \propto \exp\left(-\text{const.} \times t^{\beta\gamma}\right)$ yields the exponent relation $\beta\gamma = 1$. In the homogeneous regime, $\beta = 1$ and thus $\gamma = 1$, while in the clustering regime, $\beta = 1/2$ and thus, $\gamma = 2$.

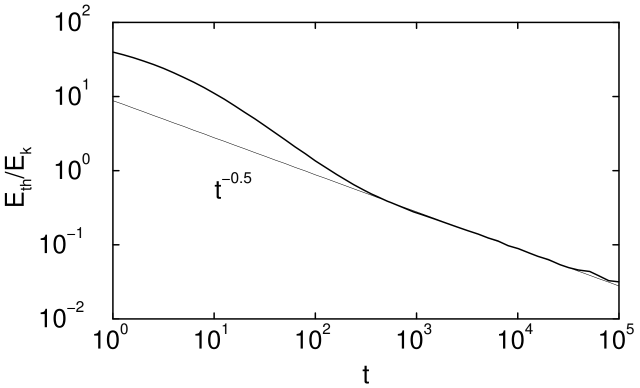

FIG. 4. The ratio of the thermal energy E_{th} to the kinetic energy E_k as a function of time for $r = 0.1$. A line of slope $-1/2$ is also shown as a reference.

To quantify collectives motions and the corresponding velocity fluctuations in the clustering regime, we also measured the local kinetic energy, E_k, and the local thermal energy, E_{th}. The local kinetic energy is defined by $E_k = \frac{1}{2}\langle \rho u^2 \rangle$ with the density ρ and the velocity $\mathbf{u} \equiv (u_x, u_y)$ obtained by averaging the corresponding quantities over a small region of space. The local thermal energy $E_{th} = \frac{1}{2}\langle (v_x - u_x)^2 + (v_y - u_y)^2 \rangle$ is obtained by subtracting the average local velocity $\mathbf{u}$ from the particle velocity $\mathbf{v}$. Space was divided into 128×128 small boxes. As shown in Fig. 4, initially, the thermal energy is large compared with the kinetic energy, indicating that particles essentially move independently and there are no collective motions. In contrast, in the asymptotic regime, $t \gg t_c(r = 0.1) \approx 10^2$ the thermal energy becomes much smaller than the kinetic energy, indicating that coherent motion of particles becomes dominant. The appearance of the collective motions was suggested by linear stability analysis of the hydrodynamic equations [2,7] and observed in MD simulations [2,3,5,7,9–13].

Interestingly, we find that the ratio of thermal to kinetic energy decays algebraically, $E_{th}/E_k \sim t^{-0.5}$, in the long time limit. The thermal energy, $E_{th} = \frac{1}{2}\langle (\Delta v)^2 \rangle$ quantifies local velocity fluctuations, Δv, and using Eq. (3),

$$E_{th} \sim (\Delta v)^2 \sim t^{-3/2}. \tag{5}$$

In other words, local velocity fluctuations, $\Delta v \sim t^{-3/4}$ are small compared with the typical velocity, $v \sim t^{-1/2}$, as $\Delta v/v \sim t^{-1/4}$. Thus, at least two distinct velocity scales are needed to characterize particle velocities in the clustering regime. Moreover, the relatively small velocity fluctuations imply strong velocity correlations and a well-defined average local velocity. Thus, a hydrodynamic description is plausible in the clustering regime.

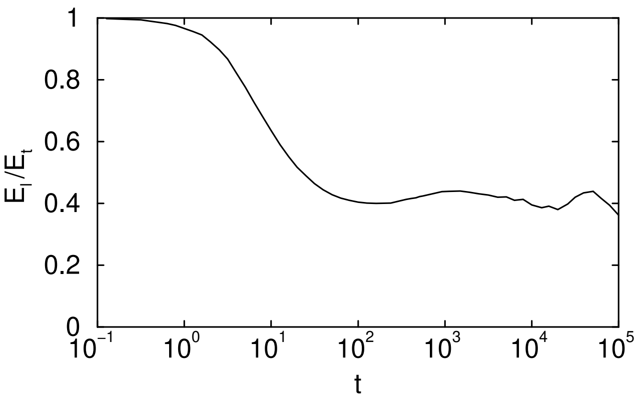

FIG. 5. The ratio of the longitudinal energy E_l to the transverse energy E_t as a function of time.

To distinguish between acoustic and shear modes, we transformed the averaged velocity field into Fourier space and decomposed the velocity as $\mathbf{u}(\mathbf{k}) = \mathbf{u}_l(\mathbf{k}) + \mathbf{u}_t(\mathbf{k})$. Here $\mathbf{u}_t(\mathbf{k})$ is the transverse velocity satisfying $\mathbf{k} \cdot \mathbf{u}_t = 0$, and $\mathbf{u}_l(\mathbf{k})$ is the longitudinal velocity with $\mathbf{k} \times \mathbf{u}_l = 0$. The corresponding representation in physical space is $\mathbf{u}(x, y) = \mathbf{u}_l(x, y) + \mathbf{u}_t(x, y)$, with $\nabla \cdot \mathbf{u}_t = 0$, and

$\nabla \times \mathbf{u}_l = 0$. The averaged longitudinal energy, i.e., the energy of acoustic modes, is defined as the spatial average $E_l = \frac{1}{2}\langle \rho u_l^2 \rangle$, and the transverse energy, i.e., the energy of shear modes, is defined as the space average of $E_t = \frac{1}{2}\langle \rho u_t^2 \rangle$. Initially, the system is isotropic and consequently, the longitudinal and the transverse energies are equal (see Figure 5). Since collective motions are negligible initially, statistical fluctuations are isotropic as well. The ratio of longitudinal to transverse energies decreases steadily and eventually, it saturates at a value of roughly $E_l/E_t \to 0.4$ for $t > t_c$. Therefore, shear modes dominate over acoustic modes in the clustering regime. This behavior is consistent with the formation of dense, thin, elongated clusters, where particles move coherently, parallel to the cluster orientation [2]. Interestingly, we did not observe obvious correlations between the cluster size and its velocity.

Collective motion of granular media can be described by mass, momentum and energy balance equations [2,7,24,25]. We have seen that the thermal energy, i.e., the temperature T, is negligible compared with the kinetic energy, and therefore, we may expand the system around zero temperature. In particular, we can ignore the pressure term in the momentum equation due to the fact that $p \sim T$ while keeping the viscosity term since $\nu \sim T^{1/2}$ [7]. The resulting governing equations are

$$\partial_t \rho + \partial_\alpha(\rho u_\alpha) = 0, \tag{6}$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = \partial_\beta \pi_{\alpha\beta}, \tag{7}$$

$$\pi_{\alpha\beta} = \partial_\alpha(\rho\nu u_\beta) + \partial_\beta(\rho\nu u_\alpha) - \partial_\gamma(\rho\nu u_\gamma)\delta_{\alpha\beta}, \tag{8}$$

taken in the limit of vanishing viscosity, $\nu \to 0$. The above equations are similar to the two-dimensional Burgers equation supplemented by the continuity equation, used to model large-scale formation of matter in the universe [26,27]. Here, the formation of shocks corresponds to dense, thin, string-like clusters where particles move parallel to the cluster orientation. At least qualitatively, this is consistent with the above findings that shear modes dominate over acoustic modes.

In conclusion, our simulations show that in the low density and large system limits, the kinetic energy of freely evolving granular media decays with time as t^{-1} in the long time limit. We have also observed that the particle velocity distribution is Gaussian in this asymptotic time regime. The above behavior is independent of the degree of dissipation. We have studied the origin of this universality and found that the asymptotic dynamics are dominated by collective motions of particles or alternatively, shear modes. In the clustering regime, strong spatial velocity correlations develop, as local velocity fluctuations are much smaller compared with the typical velocity. We have also argued that the governing continuum equations are similar to the two-dimensional Burgers equation with infinitely small viscosity.

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