A universal scaling law for the evolution of granular gases

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Abstract - Dry, freely evolving granular materials in a dilute gaseous state coalesce into dense clusters only due to dissipative interactions. Here we show that the evolution of a dilute, freely cooling granular gas is determined in a universal way by the ratio of inertial flow and thermal velocities, that is, the Mach number. Theoretical calculations and direct numerical simulations of the granular Navier-Stokes equations show that irrespective of the coefficient of restitution, density or initial velocity distribution, the density fluctuations follow a universal quadratic dependence on the system’s Mach number. We find that the clustering exhibits a scale-free dynamics but the clustered state becomes observable when the Mach number is approximately of $O(1)$. Our results provide a method to determine the age of a granular gas and predict the macroscopic appearance of clusters.

A freely cooling granular gas is an ensemble of particles undergoing dissipative collisions and free of any external field. Such granular gases have been used as model systems to describe geophysical processes such as Plinian eruptions [1,2], the solar corona [3], the asteroid belt between Mars and Jupiter, planetary rings [4,5], protoplanetary disks [6], and the formation of cosmological structures [7] because granular dissipative processes may play a role. Even a small degree of dissipation in the kinetics of granular particles produces spatial correlations and structures in a dilute, homogeneous gas [8]. Hydrodynamic treatments suggest that a shear instability initiates this transition [8]. However, when exactly this process initiates is not known.

The equations of granular hydrodynamics [9] predict a linear instability of the transverse mode [10] when the wave vector $|\vec{k}| \leq k^*_\perp(\varepsilon)$, where $k^*_\perp(\varepsilon) \propto (1 - \varepsilon^2)^{1/2}$ and $\varepsilon$ is the coefficient of restitution $\varepsilon = |u'/u|$, where $u$ ($u'$) is the normal relative velocity before (after) a collision. This instability leads to the formation of vortices. In regions where the particle velocities are correlated the temperature drops, which, in turn, creates regions of low pressure. These are the seeds for a second instability if the system size is larger than $h^{-1}_\perp(\varepsilon) > k^{-1}_\perp(\varepsilon)$. Although freely cooling granular gases have attracted wide interest [11–17], there remains, beyond issues of finite sizes, the outstanding question of what sets the rise of the density inhomogeneities. Past works made differing claims as to what the onset time of clustering is [14,16,18].

Experimental studies [19–23] of granular gases are rather scarce because of formidable challenges in preparing a system free of external forces. Microgravity experiments on parabolic flights or drop towers potentially offer good conditions, but it is very difficult to remove the influence of confining potentials or surrounding walls on the granular system.

The necessity of studying large system sizes and of characterizing fluctuations in regions of sharp gradients in temperature and density, developing into supersonic flow, without ambiguities motivates us to tackle the continuous hydrodynamic equations beyond perturbative schemes. Hydrodynamic fields can be rigorously defined in a manner similar to molecular fluids by means of a coarse-graining of the microscopic kinetic equations. First, one considers the one-particle distribution function $f(\vec{r}, \vec{v}, t)$, which obeys the Boltzmann equation and represents the number of particles within a volume $d\vec{r}$ centered at $\vec{r}$ and with velocity $\vec{v}$ within the interval $d\vec{v}$. Then, the transport equations for inelastic systems are derived by using a Chapman-Enskog expansion [24–26]. From the moments of $f(\vec{r}, \vec{v}, t)$ the number density $n(\vec{r}, t)$, convective velocity $\vec{v}(\vec{r}, t)$, and temperature $T(\vec{r}, t)$ fields can be derived. Physically, the granular temperature $T(\vec{r}, t)$ represents the fluctuations of the microscopic velocities $\vec{v}$ or, in other

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words, it is the energy of the uncoordinated motion of particles.

Direct numerical simulations (DNS) of the hydrodynamic equations give access to enlightening results because all hydrodynamic fields are accessible at each point of space and time. Therefore, DNS allow for the possibility of observing fluctuations and structure formation on scales inaccessible to molecular-dynamics (MD) simulations. In MD simulations of granular gases one has to pay attention to statistical averaging because the steadily changing average properties and the strong spatial gradients make any averaging scheme challenging. Appropriate coarse-graining techniques for MD can be found in [27–29].

We solve the compressible Navier-Stokes equations for number density $\rho$, momentum $m\vec{v}$, and $T$ of a granular gas in three dimensions. For a granular gas made of particles with diameter $\sigma$, mass $m$, average filling fraction $\bar{\phi} \equiv \frac{1}{6}\rho\sigma^3$ and coefficient of restitution $\epsilon = \text{const}$ the equations can be written in the following form [9]:

$$\begin{align*}
\partial_t \rho + \nabla \cdot (\rho \vec{v}) &= 0, \\
\frac{D}{Dt} \vec{v} + \frac{1}{\rho m} \nabla \cdot \left\{ \rho \vec{v} (\nabla \vec{v})^T - \left( \frac{2}{3} \nabla \cdot \vec{v} \right) \mathbf{1} \right\} &= 0, \\
\frac{D}{Dt} T - \frac{2}{3\rho} \rho \vec{v} \cdot \nabla \bar{\phi} + \frac{2}{3\rho} \nabla \cdot \vec{q} + \xi T &= 0,
\end{align*}$$

where $\partial_t \equiv \partial/\partial t$, and $D/Dt \equiv \partial_t + (\vec{v} \cdot \nabla)$ is the material derivative; in eqs. (1)–(3) the hydrostatic pressure $p$ and the heat flux $\vec{q}$ are given by

$$p = \rho T \left[ 1 + \frac{1+\epsilon}{3} \rho \sigma^3 g_2(\rho) \right],$$

$$\vec{q} = -\kappa \nabla T - \mu \nabla p.$$

The transport coefficients are viscosity $\eta = \eta(T^{1/2} g_2^{-1})$, thermal conductivity $\kappa = \kappa(T^{1/2} g_2^{-1})$, the coefficient $\mu = \mu(T^{3/2} \rho^{-1} g_2^{-1})$ [30,31], the cooling factor $\xi = \xi(\rho T^{1/2} g_2)$, and the pair correlation function $g_2 = g_2(\rho)$; further details on these equations can be found in [9,32]. The heat flux for granular materials contains a "pycnothermal" term $\mu$, that is a density-thermal-flux coupling, in addition to thermal gradients [30]. The term proportional to the density gradient is in principle present also in molecular fluids but the Onsager theorem protects against it [33], yielding $\mu = 0$. In contrast, for granular gases the coarse-graining of particles’ degrees of freedom that generates hydrodynamic fields produces a non-vanishing $\mu$ [34].

We also include the Carnahan-Starling pair-correlation function

$$g_2(\phi) = \frac{(2 - \phi)}{(2(1 - \phi))^3}$$

to realistically represent spatial correlations for finite-size particles, where $\phi \equiv \frac{1}{6}\rho\sigma^3$ is the local filling fraction$^1$.

We solve eqs. (1)–(4), similarly to what is conventionally done for molecular fluids, for the dimensionless, conservative variables $\rho, \rho\vec{v}, \rho E$, with $E = \vec{v}^2 + T$. We measure time in units of $\sigma/\nu_{th,0}$, where $\nu_{th,0}$ is the initial value of $\sqrt{2T}/3$, and set $m = 1$. We employ a finite-volume method on a grid of $128^3$ cells with periodic boundary conditions. The granular Navier-Stokes equations in conservative form are integrated in each grid cell. Because of the Gauss theorem the volume integrals become surface integrals in each cell. Each surface integral is performed via 4 Gaussian stencils. We perform an operator splitting to calculate the convective and the diffusive fluxes, and the source terms independently. The interpolation of the variables needed at the Gaussian stencils is performed via a seventh-order WENO method [36,37] and the flux is approximated with the help of a MUSTA scheme [38]. The time integration is carried out explicitly with a third-order Runge-Kutta TVD scheme [39]. The diffusive flux is calculated via an implicit Euler method. The entire solver was implemented on a Nvidia’s TESLA K20c GPU accelerator with a CUDA code. Hydrodynamic simulations have been shown to reproduce results from molecular-dynamics simulations [40–42].

Figure 1 shows the evolution of $p(\vec{r},t)$ and $T(\vec{r},t)$ in a freely cooling gas. We observe that out of the homogeneous cooling state small, cold regions of larger density emerge throughout the system and grow in size with time. The high-density regions (clusters) are filamentous because of the shear instability. The morphology of the clusters we find in our simulations agrees with the shape of the clusters which have been seen in MD simulations [43,44]; however, our system size allows the formation of multiple, large clusters. We quantify the cluster growth by calculating the maximum filling fraction $\phi_{\text{max}}$ and the density fluctuations $(\langle \delta \rho \rangle^2) = \frac{1}{L^3} \langle (\delta \phi)^2 \rangle$ across the system, which allows one to compare systems with different average filling fractions $\phi$. Hereafter the angle brackets indicate spatial averaging over the entire system. Figure 2 shows the temporal evolution of these quantities. In the homogeneous cooling state $\phi_{\text{max}}$ is very small, but suddenly the system develops inhomogeneities. Figure 2(b) reveals an early-time dynamics not directly accessible when observing the maximum filling fraction (fig. 2(a)). What appears to be a sudden emergence of clusters at characteristic times depending on $\epsilon$ in fig. 2(a) is instead a scale-free process described by a power law $\sim t^\alpha$, with $\alpha \approx 1.85$. Thus, if the signal-to-noise ratio

$^1$All simulations are stopped once the maximum local filling fraction $\phi_{\text{max}}$ is 5% above the average filling fraction $\bar{\phi}$; this ensures that our calculations remain in a regime where the pair correlation function holds. $\phi_{\text{max}}$ is the maximum value of all local filling fractions $\phi_i$ in the system. The results of this work are valid until the time when the granular system starts forming dense clusters. For further discussion on the validity and limits of the equations of state see [55].
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Fig. 1: (Color online) Snapshots of the system showing the temporal evolution of a three-dimensional granular gas with a coefficient of restitution $\varepsilon = 0.9$ and average filling fraction $\bar{\phi} = 0.05$. Top row: from left to right, snapshots of the density field at times $t = 10^9$, $t = 10^{10}$ and $t = 10^{11}$, respectively. Darker regions represent larger local average density. Bottom row: three-dimensional map of the temperature field $T(\vec{r}, t)$ at the same times of the corresponding density plot in the top row. The color (red: hot; blue: cold) represents the local temperature compared to the average temperature in the system.

Fig. 2: (Color online) Temporal evolution of the maximum filling fraction $\phi_{\text{max}}$ (a) and of the filling fraction fluctuations $\langle (\delta \phi)^2 \rangle$ (b). In (a) the average filling fraction is $\bar{\phi} = 0.05$. The clustering process exhibits the same qualitative features over a wide range of coefficients of restitution $\varepsilon$ and average filling fractions $\bar{\phi}$. The curves are guides to the eye. As $\varepsilon$ grows, the time of onset of clustering increases of four orders of magnitude. The inset panel shows the effect of varying average filling fractions. The initial crossover at $\langle (\delta \phi)^2 \rangle \approx 10^{-16}$ is an effect of the initial transient.

of the measurements is not large enough, an apparent sudden onset of clustering will be visible only when $\phi_{\text{max}}$ has reached few percent. To understand the origin of the increase of the density we examine the behavior of the average kinetic energy $E_{K_{\text{in}}} \equiv \sum_i \rho_i \vec{v}_i^2 / \sum_i \rho_i$ and the average temperature $T \equiv \sum_i \rho_i T_i / \sum_i \rho_i$, where $i$ is the index of the finite volumes, and compare it with the temporal evolution of $\langle (\delta \phi)^2 \rangle$. The temperature follows Haff’s law $T(t) = T_0 (1 + t/\tau)^{-2}$, $\tau \propto \hat{\phi} (1 - \varepsilon^2) \sqrt{T_0}$, while $E_{K_{\text{in}}}(t)$ decays with time in a much weaker way. Figure 3 shows that the size of the inhomogeneities is directly linked to the relative decrease of the kinetic energy $E_{K_{\text{in}}}(t)$ with respect to the temperature. In fact, when the kinetic energy equals the temperature (Haff’s law), $\langle (\delta \phi)^2 \rangle$ reaches the same value $\approx 10^{-4}$ for all our simulations. This point coincides with the time when clusters would become
visible in an experiment or molecular-dynamic simulation (i.e. $\Delta \phi \sim \sqrt{\langle (\delta \phi)^2 \rangle} \approx 1\%$). Therefore, it seems appropriate to us to consider the Mach number $\mathcal{M} \equiv \sqrt{\langle v^2 \rangle / T}$ as a scaled measure of the granular dynamics. The granular gas develops visible clusters when $\mathcal{M}$ is of the order of unity, that is the threshold of supersonic flow. Changing the average filling fraction or coefficient of restitution does not alter this conclusion. We note that Haff’s law is derived under the assumption of no macroscopic fluxes and homogeneous density [45]. Because of these assumptions it is not possible to conclude anything about either the density or the velocity fluctuations out of Haff’s law. In the context of our definition of the Mach number, Haff’s law assumes $\mathcal{M} \equiv 0$.

Because the system is translational invariant and there is no characteristic time scale associated with the condition $\mathcal{M} \sim \mathcal{O}(1)$, we expect the evolution of the freely cooling gas to be scale invariant when described with the relevant variables. In fact, under general assumptions we can prove with an analytical argument that the density fluctuations $\langle (\delta \rho)^2 \rangle$ scale quadratically with $\mathcal{M}$. We assume that: i) the granular gas is in a homogeneous cooling state where Haff’s law holds, $T = T_0 (1 + t/\tau)^{-2}$, and the density fluctuations are still small, that is, $\delta \rho \ll \overline{\rho}$; ii) isotropy of the velocity, $v_{ix} = v_{iy} = v_{iz}$; iii) the equation of state of ideal gases holds: $p = \rho T$; iv) the system is so large that we can neglect finite-size effects and that diffusion is negligible; v) local convective fluxes and their gradients are small: $v_i \partial_i v_j \ll T^{1/2}$, $i,j \in \{x,y,z\}$. Equations (1), (2) then become

$$\partial_t \rho + \nabla \cdot (\rho \vec{v}) = 0,$$

$$\partial_t \vec{v} + \frac{1}{\rho} \nabla (\rho T) = 0. \quad (7)$$

We start by multiplying eq. (6) by $\rho^{-1}$ and taking the spatial average over the volume $\Omega$, $\langle \Phi \rangle \equiv \frac{1}{\Omega} \int_\Omega \Phi \mathrm{d}\Omega$. We consider fluctuations around the homogeneous background solution $\rho$, so that we can write

$$\partial_t \langle \log(\rho) \rangle = \partial_t \langle \log(\rho) \rangle + \partial_t \langle \delta \rho \rangle/\bar{\rho} - \frac{1}{2} \partial_t \langle (\delta \rho)^2 \rangle/\bar{\rho}^2 + \mathcal{O}(\delta \rho^3/\bar{\rho}^3)$$

$$= - \frac{1}{2} \partial_t \langle (\delta \rho)^2 \rangle/\bar{\rho}^2 + \mathcal{O}(\delta \rho^3/\bar{\rho}^3). \quad (8)$$

The surface integral $\langle \nabla \cdot \vec{v} \rangle$ vanishes. Using eq. (8), eq. (6) becomes

$$- \frac{1}{2} \partial_t \langle (\delta \rho)^2 \rangle/\bar{\rho}^2 + \mathcal{O}(\delta \rho^3/\bar{\rho}^3) = 0. \quad (9)$$

We now take the scalar product of eq. (7) with $\vec{v}$, followed by the space averaging, which yields

$$\frac{1}{2} \partial_t \langle v^2 \rangle + T \langle \vec{v} \cdot \nabla \bar{\rho} \rangle = 0, \quad (10)$$

where we assumed that the spatial dependence of $T$ is negligible. Equations (9) and (10) lead to

$$\frac{\langle (\delta \rho)^2 \rangle}{\bar{\rho}^2} = - \int \frac{\partial_t \langle v^2 \rangle}{T} dt + \text{const.} \quad (11)$$

Haff’s law predicts that $T = T_0 (\tau/t)^{-2}$ for $t \gg \tau$, which we insert into eq. (11). From our simulations we find out that the kinetic energy follows also a power law $\bar{\rho}^{-2} = s (t^\gamma, A \approx 0.07$ (see fig. 3(a)). Combining this result with eq. (11) we find

$$\frac{\langle (\delta \rho)^2 \rangle}{\bar{\rho}^2} \propto \frac{A}{2 - A} \mathcal{M}^2 + \text{const.} \quad (12)$$

Figure 4 collects results from extensive DNS calculations where we varied $\varepsilon$, the initial value of the Mach number $\mathcal{M}_0$ and $\phi$, and shows the evolution of $\langle (\delta \phi)^2 \rangle$ in terms $\mathcal{M}$. Regardless of the system parameters or the initial state, the density fluctuations converge onto the locus $\langle (\delta \phi)^2 \rangle(\mathcal{M}) = c \mathcal{M}^2$, where $c$ is a constant. This universal scaling is robust also upon variation of the initial conditions.

The locus $\langle (\delta \phi)^2 \rangle = c \mathcal{M}^2$ plays the role of an “attractor” for the evolution of the granular gas, as is visible from fig. 4: when the initial Mach number $\mathcal{M}_0$ is large, the system shows a weak transient decrease of $\mathcal{M}_0$, due to a relaxation of the initial condition, which is then followed by the approach and collapse onto the locus $\langle (\delta \phi)^2 \rangle = c \mathcal{M}^2$. Once the initial conditions are forgotten,
all systems investigated show universal behavior, as visible from the collapse of all curves in fig. 4 over several decades. The universal power-law behavior of a granular gas in the homogeneous cooling state indicates that there is no characteristic time scale for the onset of clustering. However, because of finite resolution, an experiment would observe the onset of clustering when $M \sim O(1)$.

For reasons of computational convenience our DNS are based on the simplified model assuming $\varepsilon = \text{const}$, that is, $\varepsilon$ is a material property. However, it is known that in reality $\varepsilon$ depends on the impact velocity $u$ [5]. In more realistic models particles are treated as viscoelastic spheres [46–48]. Therefore, the question naturally arises as to whether our results depend on the model of the collisional kinetics. In fact, we have implemented a model of viscoelastic spheres as described in [9,47,49,50]. For reasons of computational convenience we have tested the general validity of our arguments in two spatial dimensions\(^2\). The inset of fig. 4 shows that DNS for $\varepsilon = \text{const}$ and $\varepsilon = \varepsilon(u)$ reproduce the same scaling behavior of the density fluctuations in terms of the Mach number, though the prefactor depends on the dimensionality of the system.

It is important to note at this point that our heuristic derivation makes explicit use of Haff’s law, written generally as

$$T(t) = T_0 \left( 1 + \frac{t}{\tau} \right)^{-\alpha}, \quad (13)$$

where $\tau$ is the characteristic cooling time [49] and $\alpha = 2$ if $\varepsilon = \text{const}$, or $\alpha = 5/3$ if $\varepsilon = \varepsilon(u)$, that is, in the viscoelastic model. Importantly, although the scaling exponents of the two models differ, our analytical arguments produce in both cases the quadratic dependence of density fluctuations on the Mach number. We can thus conclude that our main findings do not depend on the details of the collisional kinetics.

The results of the current work might provide a tool to measure the age of such granular gases in the context of the Mach number. It might also lead to a prediction of the lifetime of protoplanetary accretion discs, that is their disappearance when macroscopic clustering takes place. In the geophysical context, our results could help improve models of pyroclastic density currents [2]. Possible future improvements might be provided by coupling hydrodynamic models with particle-based simulations. In summary, we have shown by means of DNS and theoretical calculations that i) the dynamics of a freely cooling granular gas follows a universal power-law behavior in terms of the ratio of convective to thermal velocities, irrespective of the initial state, and ii) the onset of clustering has no characteristic time scale.

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