Declustering in a granular gas as a finite-size effect

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The existence of dense clusters has been shown to be a transient phenomenon for realistic models of granular collisions, where the coefficient of restitution depends on the impact velocity. We report direct numerical simulations that elucidate the conditions for the disappearance of structures. We find that upon cluster formation the granular temperature and the convective kinetic energy couple and both follow Haff's law. Furthermore, we show that clusters will eventually dissolve in all finite-size systems. We find the strong power law $t' \propto L^{12}$ for the dependency of the declustering time on system size. Our results imply that only in systems close to the initial critical system size both clustering and declustering transitions are observable.

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Clustering transitions in granular systems are ubiquitous processes in astrophysical [1–4] and geophysical settings [5–7]. Additionally, granular gases have become a paradigmatic example of nonequilibrium statistical physics [8].

In granular collisions, the component of the relative velocity of the colliding particles along the line joining the two centers of mass, $|\vec{u}|$, decreases in absolute value by a factor $0 < \varepsilon < 1$, called the coefficient of restitution. Thus, in the absence of convective fluxes, the average kinetic energy of the system (granular temperature) steadily decreases. The temperature of a homogeneous granular gas, with initial temperature T_0, follows Haff's law:

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

where t is the time, τ the characteristic cooling time [9], and $\alpha = 2$ if $\varepsilon = \text{const}$. This cooling process is well understood in theory [10], simulations [11–15], and experiments [16–20]. If the system size L is larger than a critical size

$$L_{\text{crit}} \propto (1 - \varepsilon^2)^{-1/2}, \tag{2}$$

a transition from the homogeneous cooling state (HCS) into an inhomogeneous cooling state (ICS) [21,22] appears, which is characterized by the formation of dense clusters [11–15,23–25]. However, in reality ε depends on the impact velocity u [3]. In a more realistic model particles are treated as viscoelastic spheres [26–28] and

$$\varepsilon(u) = 1 - \gamma|u|^{1/5} + \tfrac{3}{5}\gamma^2|u|^{2/5} \mp \cdots, \tag{3}$$

where γ is a constant depending on material properties. The enormous decrease of granular temperature during the cooling process leads to a drastic decrease of the energy dissipation $(1 - \varepsilon^2)$, which makes the assumption $\varepsilon = \text{const}$ unrealistic. For a realistic granular gas [$\varepsilon = \varepsilon(u)$] the slope of Haff's law is $\alpha = 5/3$ [27] and it has been shown that the clustering is a transient phenomenon [29,30]. Here we show that the disappearance of clusters in granular gases is in principle a finite-size effect. As the granular temperature decreases, the critical system size increases until it reaches the size of the system, upon which the density inhomogeneities dissolve and the system returns to a homogeneous state. However, the steep dependence of the time of homogenization on system size implies that for any amount of dissipation a system size can be found where the gas will remain heterogeneous at any realistic time scale.

To study large system sizes and characterize fluctuations in regions of sharp gradients in temperature and density, which develop into supersonic flow, without ambiguities, we employ the continuous hydrodynamic equations beyond perturbative schemes. Hydrodynamic fields can be rigorously defined in a manner similar to molecular fluids by means of a granular Boltzmann transport equation [31–33]. From the moments of the one-particle distribution function $f(\vec{r},\vec{w},t)$ the number density $\rho(\vec{r},t)$, convective velocity $\vec{v}$, and temperature $T(\vec{r},t)$ fields can be derived for each space-time point $(\vec{r},t)$. Physically, $T(\vec{r},t)$ represents the fluctuations (second moment) of the microscopic velocities $\vec{w}$. The resulting Navier-Stokes equations for granular gases for $\varepsilon = \text{const}$ [34] and for viscoelastic particles [35] have the same functional form.

In two dimensions, the Navier-Stokes equations for a granular gas made of particles with diameter σ, mass m, and coefficient of restitution $\varepsilon = \varepsilon(u)$ can be written in the following form [29]:

$$\begin{aligned}
&\partial_t\rho + \nabla\cdot(\rho\vec{v}) = 0\\
&\frac{D}{Dt}\vec{v} + \frac{1}{\rho m}\nabla\cdot\{p\mathbf{1} - \eta[\nabla\vec{v} + (\nabla\vec{v})^T - (\nabla\cdot\vec{v})\mathbf{1}]\} = 0\\
&\frac{D}{Dt}T - \frac{1}{\rho}\eta\{[\nabla\vec{v} + (\nabla\vec{v})^T - (\nabla\cdot\vec{v})\mathbf{1}] : \nabla\vec{v}\}\\
&\quad + \frac{1}{\rho}p\nabla\cdot\vec{v} + \frac{1}{\rho}\nabla\cdot\vec{q} + \xi T = 0,
\end{aligned} \tag{4}$$

where $D/Dt \equiv \partial_t + (\vec{v}\cdot\nabla)$ is the material derivative and $\mathbf{1}$ is the unit tensor; the hydrostatic pressure p and the heat flux $\vec{q}$ are given by

$$\begin{aligned}
p &= \rho T\left[1 + \frac{1+\varepsilon}{4}\rho\pi\sigma^2 g_Q(\phi)\right],\\
\vec{q} &= -\kappa\nabla T - \mu\nabla\rho.
\end{aligned} \tag{5}$$

The transport coefficients are viscosity $\eta = \eta(T, g_Q)$, thermal conductivity $\kappa = \kappa(T, g_Q)$, the coefficient

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$\mu = \mu(T,\rho,g_Q)$, and the cooling factor $\xi = \xi(T,\rho,g_Q)$ [34], and $g_Q = g_Q(\phi)$ is the pair correlation function which depends on the filling fraction $\phi \equiv \frac{1}{4}\rho\pi\sigma^2$; further details to these equations can be found in [29]. We employ the transport coefficients for the $\varepsilon = \text{const}$ model [34]. We discuss below the validity of this assumption. The heat flux for granular materials contains a "pycnothermal" term, that is, a density-thermal-flux coupling, in addition to thermal gradients [36]. The term proportional to the density gradient is in principle present also in molecular fluids but the Onsager theorem protects against it [37], yielding $\mu = 0$. In contrast, for granular gases the coarse-graining of particles' degrees of freedom that generates hydrodynamic fields produces a nonvanishing μ [38].

We perform direct numerical simulation (DNS) of the hydrodynamic equations in two dimensions with periodic boundary conditions on a 128×128 grid. We choose the linear system size L in units of σ, and the initial thermal velocity $v_{T,0}$ as reference velocity, which means that the temperature is measured in units of $\frac{1}{2}mv_{T,0}^2$. We employ Luding's global, two-dimensional (2D) pair correlation function g_Q [39]:

$$g_Q = g_4 + n(\phi)(g_{\text{dense}} - g_4), \tag{6}$$

where

$$g_4 = \frac{1 - 7/16\phi}{(1-\phi)^2} - \frac{\phi^3}{128(1-\phi)^4},$$

$$n(\phi) = \left[1 + \exp\left(\frac{\phi_c - \phi}{\alpha_\phi}\right)\right]^{-1},$$

$$g_{\text{dense}} = \frac{\phi_m}{\phi}\left((\phi_m - \phi)^{-1} + c_1 + c_3(\phi_m - \phi)^2 - \frac{1}{2\phi_m}\right),$$

with the maximum packing fraction $\phi_m \equiv \frac{\pi}{2\sqrt{3}}$, the transition point $\phi_c = 0.6990$, and fitting parameters $c_1 = -0.04$, $c_3 = 3.25$, and $\alpha_\phi = 0.0111$. The pair correlation function g_Q is valid for all densities in two dimensions and leads to a global equation of state which diverges not more than 1% from results of molecular dynamics (MD) simulations [39,40]. The maximum deviation appears during the transition regime at $\phi \approx \phi_c$; apart from this transient regime the error margin is smaller than 0.1%. Finally, we assume that the thermal velocity $v_T = T^{1/2}$ defines the local ε. To calculate the variable coefficient of restitution, $\varepsilon(u)$, we truncate Eq. (3) after the linear term and assume that the impact velocity is equal to the thermal velocity $T^{1/2}$. This is a mean-field-like approximation. This implies that we use a quasi-two-dimensional model because Eq. (3) was strictly derived for spheres and not hard disks [26–28]. We use an integration time step δt small enough so that even in the viscoelastic model $\varepsilon \approx$ const during a δt. For reasons of self-consistency we then use the transport coefficients in [34], where, however, $\varepsilon = \varepsilon(T(\vec{r},t))$. We have compared our results with the full viscoelastic model [35] and do not observe any qualitative or significantly quantitative difference. We solve Eqs. (4) and (5) by using a finite-volume discretization. We use an operator splitting method for the convective and diffusive flux, and for the temperature sink [41]. The Riemann problem, which appears during the calculation of the convective flux, is solved with a multistage ansatz (MUSTA) [42] and the diffusive flux is calculated via an implicit Euler scheme. For all

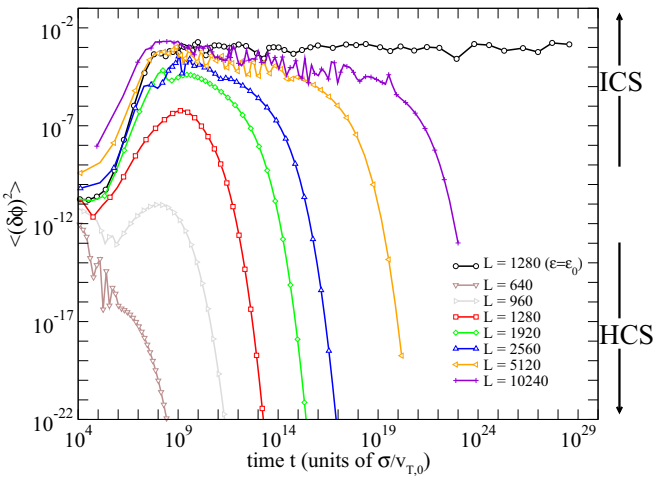

FIG. 1. Temporal evolution of density fluctuations in 2D granular gases with an average filling fraction $\bar{\phi} = 0.05$. The black circles correspond to calculations at constant $\varepsilon = 0.99$. All other symbols correspond to calculations for viscoelastic particles where $\varepsilon_0 = \varepsilon(t = 0) = 0.99$. The critical system size for this ε_0 is $L_{\text{crit}} \approx 500$. If the system is large enough, the fluctuations grow until the clustering becomes visible. For a constant ε the fluctuations reach a plateau. When $\varepsilon = \varepsilon(T)$ the fluctuations first grow to a size-dependent maximum but eventually vanish after a certain time. This time grows with system size.

necessary integrations we use a two-point Gaussian-Legendre integration in each dimension, and for the interpolation of the hydrodynamic variables and their derivatives we use the weighted essentially non-oscillatory (WENO) reconstruction of seventh and sixth order, respectively [43].

We quantify the degree of clustering by calculating the density fluctuations $\langle(\delta\rho)^2\rangle = \frac{1}{\bar{\phi}^2}\langle(\delta\phi)^2\rangle$ across the system, where $\bar{\phi}$ is the average filling fraction. Figure 1 shows the evolution of the density fluctuations for systems having the same initial ε but differing in size. For constant $\varepsilon = 0.99$ the density fluctuations reach a plateau value of about 5×10^{-3}. The density fluctuations for $\varepsilon = \varepsilon(T)$ also reach typical values, but only as intermediate states. They always decay to vanishing values, but with a characteristic time t^* that depends on the system size. To avoid natural fluctuations in the degree of clustering we define t^* as the time when $\langle(\delta\phi)^2(t^*)\rangle = 10^{-20}$. Figure 2 shows the dependence of t^* on the linear size of the system. Except for the smallest size investigated, the calculations are well fit by a power law with the rather large exponent of 12.

It is useful for our discussion below to also consider the temporal evolution of the average kinetic energy of the system, $E_{\text{kin}} \equiv \Sigma_i \rho_i \vec{v}_i^{\,2} / \Sigma_i \rho_i$, and the average temperature $T \equiv \Sigma_i \rho_i T_i / \Sigma_i \rho_i$, where i is the index of the finite volume. Figure 3(a) shows the evolution of E_{kin} and T for a gas with $\varepsilon =$ const, and Fig. 3(b) the same quantities for a gas of viscoelastic particles [$\varepsilon = \varepsilon(T)$]. Haff's law with the appropriate α is recovered for both models. We observe two temporal regimes when $\varepsilon =$ const: a HCS when T follows Haff's law and E_{kin} follows a power law with a very small exponent, and an ICS when the two curves meet and E_{kin} displays a dynamical transition to a Haff-like dependence. The transition from HCS

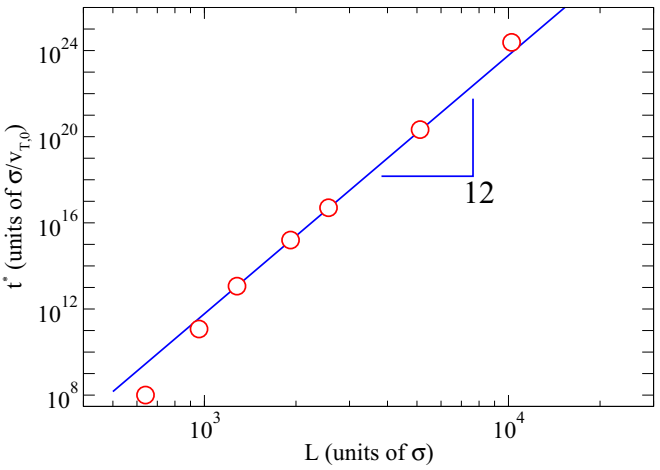

FIG. 2. The time t^* characterizing the disappearance of clusters grows with the size of the system. Results from DNS calculations are shown as circles. The solid line represents a power law with exponent 12. The value of t^* for the smallest L does not fall on the power law because the ICS is not fully developed (compare with Fig. 1).

to ICS occurs when convective and thermal velocities are of the same order of magnitude [44]. The Mach number has been shown to capture the dynamical evolution of the HCS [44]. These two quantities remain coupled for the entire remaining evolution of the gas. The beginning of the second regime marks also the transition from the HCS to the ICS with the clustering of the gas. For the model of viscoelastic particles, three temporal regimes can be recognized. Similarly to the previous case the gas starts from a HCS and transitions into an ICS which is also characterized by the coupling of $E_{\rm kin}$ and T. In the third regime, $E_{\rm kin}$ and T decouple and this coincides with the moment when the system becomes homogeneous again.

We are now in a position to rationalize the finite-size dependence of t^* with a heuristic argument in the following way. For short time intervals, the typical impact velocities will not change significantly. Hence, one can use the present value of ε to define a time-dependent $L_{\rm crit}$ as in Eq. (2). It is useful to introduce the dimensionless quantity $\ell \equiv \frac{L}{L_{\rm crit}}$. Because $L_{\rm crit}$ diverges as $\varepsilon \to 1$, ℓ vanishes. We are interested in the time t' when $\ell \approx 1$, which corresponds to the onset of declustering [see the transition to regime III in Fig. 3(b)]. We can then write $\ell = 1 = L(1-\varepsilon^2)^{1/2}$. To first order, the coefficient of restitution for viscoelastic particles depends on temperature as $\varepsilon = 1 - (1-\varepsilon_0)T^{1/10}$, where $\varepsilon_0 = \varepsilon(t=0)$ and $\gamma = 1-\varepsilon_0$. Keeping only terms of first order in $T^{1/10}$, the condition $\ell \approx 1$ leads to the relation $L^{-2} \approx (1-\varepsilon_0)T^{1/10}$. We know from Fig. 3 that Haff's law holds also in the ICS. We can then use its large time approximation for the case of viscoelastic particles, $T \approx t^{-5/3}$. Putting all together we find the power law

$$t' \propto L^{12}. \tag{7}$$

Because the late-time evolution of $\langle(\delta\phi)^2\rangle$ is well approximated by a power law (see Fig. 1) we can safely conclude that $t^* \propto t'$, which then matches our DNS calculation in Fig. 2. Equation (7) implies that the declustering transition for viscoelastic particles has no typical time scale but is instead a finite-size effect.

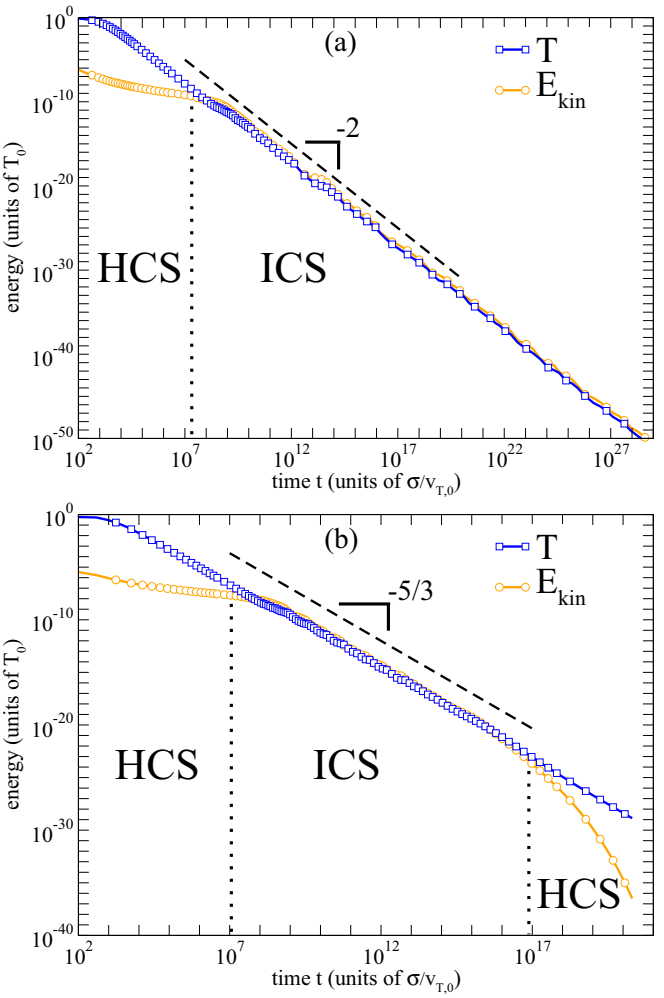

FIG. 3. Temporal evolution of the average kinetic energy $E_{\rm kin}$ and the average granular temperature T for a granular gas with average filling fraction $\bar{\phi} = 0.05$. (a) Granular system with fixed coefficient of restitution, $\varepsilon = 0.99$, and $L = 1920$. (b) Granular system with variable coefficient of restitution and initial value $\varepsilon_0 = \varepsilon(t=0) = 0.99$ and $L = 5120$. The clustering appears at the crossover of thermal energy and kinetic energy of convective velocities. In both cases thermal and kinetic energy couple at the transition point and undergo a Haff's cooling afterwards. In the case of viscoelastic particles, we can observe a decoupling of thermal and kinetic energy, which sets the onset point of declustering.

To study more closely this transition due to finite-size effects we focus on systems with $\varepsilon = \text{const}$ close to the $\ell \approx 1$ point. Figure 4 shows the density fluctuations at long times at $\varepsilon = 0.9$ and $\varepsilon = 0.999$ for different values of the dimensionless parameter ℓ. We find a sharp transition at $\ell \approx 1$ from a homogeneous gas with no clusters to a system which exhibits clusters, as expected from linear stability analysis [22]. However, linear stability analysis cannot predict the asymptotic density and size of the clusters. We find that the asymptotic cluster densities are smaller than the maximum packing fraction and their fluctuations exhibits system-size-dependent, characteristic values. The inset of Fig. 4 shows that the growth of the clusters is not unbounded but instead scales approximately linearly with the system size.

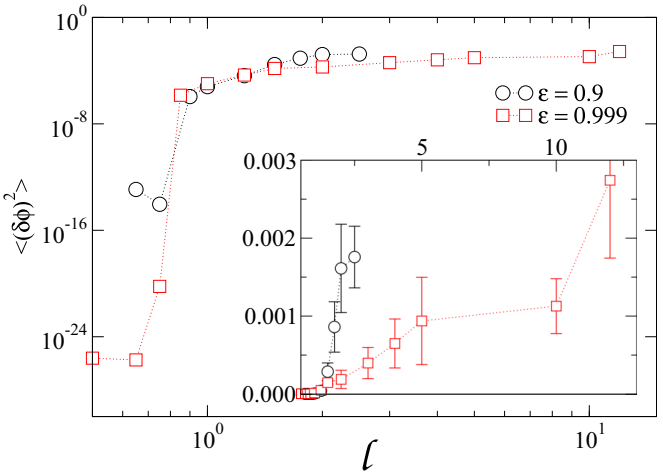

FIG. 4. Asymptotic value of the fluctuations in the ICS as a function of relative system size to the critical size $\ell \equiv L/L_{\text{crit}}$. For a fixed coefficient of restitution the fluctuations reach values that depend on the system size. The plot shows simulations for $\varepsilon = 0.9$ and $\varepsilon = 0.999$ and $\bar{\phi} = 0.05$. The inset shows the same data on a linear scale.

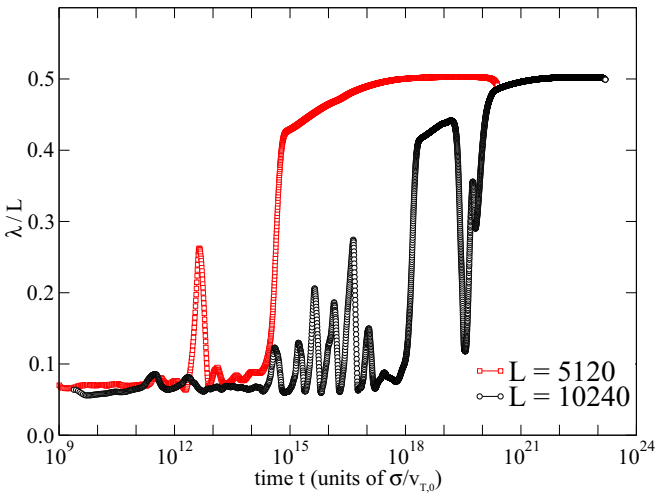

FIG. 5. Typical length of the clusters during the inhomogeneous cooling process for $\varepsilon(t = 0) = 0.99$ and $L = 5120$ and $L = 10\,240$. The values fluctuate and grow until they reach values above 0.5. The time at which this value is reached corresponds to the disappearing of clusters in the system (see Fig. 1). We calculate the length scale λ from the first moment of the Fourier transform of the density correlation function.

We report here that systems close enough to the critical system size cluster to an asymptotic packing fraction $\phi_A < \phi_m$; that is, the system does not undergo a density collapse to the maximum packing fraction.

To characterize the clusters we show their typical length scale λ in Fig. 5. The question if the declustering can appear before the size of the clusters reaches the order of the system size is of fundamental importance to the question if the declustering is a finite-size effect. Comparison of Fig. 5 and Fig. 1 reveals that the disappearance of clusters occurs not before the characteristic fluctuation size reaches 0.5. That means that declustering does not occur before the size of the clusters reaches the order of the system size. From MD simulations and linear stability analysis of the hydrodynamic equations it is known that in a granular gas with $\varepsilon = \text{const}$ the clusters grow in size until they reach the size of the system [13,14]. For variable ε the same behavior has been observed in MD simulation, if Eq. (3) holds for any u [30]. In a simplified model where $\varepsilon = 1$ for impact velocities below a threshold value the clusters dissolve before reaching the system size [45–47]. However, hydrodynamic simulation in [30] showed a cluster growth until the system size was reached for variable ε as well.

In summary, we have shown the finite-size character of the decaying of clusters in a freely cooling granular gas of viscoelastic particles. We clarified that the disappearing of density fluctuations does depend only on the size of the system. The decay time follows such a strong power law, $t' \sim L^{12}$, that only in systems close to the initial critical system size is it realistically possible to observe both the clustering and declustering transitions. Thus, for any amount of dissipation $(1 - \varepsilon^2)$ in the system, one can find a system size at which the clusters will appear as stable for an exceedingly long time. On the other hand, our results show that close to $\ell \gtrapprox 1$ the degree of clustering is extremely weak (see Fig. 4), which poses the challenge to find a system size that is large enough to observe the transition from HCS to ICS, but also small enough to observe the second transition (from ICS back to HCS) on a realistic time scale. Finally, these results indicate that an infinitely large system will not decluster.

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