Transient Structures in a Granular Gas

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A force-free granular gas is considered with an impact-velocity-dependent coefficient of restitution as it follows from the model of viscoelastic particles. We analyze structure formation in this system by means of three independent methods: molecular dynamics, numerical solution of the hydrodynamic equations, and linear stability analysis of these equations. All these approaches indicate that structure formation occurs in force-free granular gases only as a transient process.

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Cluster and vortex formation in force-free granular gases is a most striking phenomenon which makes these systems so distinct from gases of *elastic* particles, like molecular gases. First detected and explained by Goldhirsch and Zanetti [1] and McNamara [2], clustering and later vortex formation [3] have been intensively studied (e.g., [3–5]). Clustering has been also reported in recent simulations of the hydrodynamic equations [6]. In all these studies the simplifying assumption of a constant coefficient of restitution ε has been used.

It is known, however, that the coefficient of restitution is not a material constant but a function of the impact velocity, which for the most simple model of viscoelastic spheres [7] reads

$$\varepsilon(g) = 1 - \gamma|g|^{1/5} + (3/5)\gamma^2|g|^{2/5} \mp \cdots. \qquad (1)$$

Here g is the normal component of the impact velocity, and γ is a known function of the particles' material properties [7]. The typical value of ε, corresponding to the thermal velocity $v_T = \sqrt{2T(t)/m}$ [$T(t)$ is the temperature of the gas and $m = 1$ is the particle mass] behaves as $\varepsilon_T \sim 1 - \gamma T^{1/10}$; i.e., it tends to the elastic limit, $\varepsilon \to 1$, as the gas cools down, $T \to 0$.

Since a force-free gas of elastic particles tends to be homogeneous, one can naively assume that a granular gas of viscoelastic particles tends to be finally uniform as well. However, this is not necessarily true: The collisions become perfectly elastic only in the limit $g = 0$ when all particles are at rest. If the gas cools down too fast the residual structures may get frozen and persist due to a lack of kinetic energy. We illustrate this for a more general model of $\varepsilon(g)$, with $(1 - \varepsilon_T^2) \sim T^\beta$. The cooling rate of such gas is estimated as $\dot{T} \sim -n(1 - \varepsilon_T^2)T^{3/2} \sim -nT^{3/2+\beta}$ [1,8], where n is the gas number density. The gas density decreases with time due to cluster growth. If we assume $n \sim t^{-\alpha}$ $(0 < \alpha < 1)$ [9], we obtain the estimate for the gas temperature, $T \sim t^{-z}$, $z = 2(1 - \alpha)/(1 + 2\beta)$, and for the gas pressure, $P = nT \sim t^{-\alpha - z}$. If $T_{\rm cl}$ and $n_{\rm cl}$ are, respectively, the temperature and number density inside the clusters, similar estimates yield $\dot{T}_{\rm cl} \sim -n_{\rm cl}T_{\rm cl}^{3/2+\beta}$. Assuming that $n_{\rm cl}$ keeps approximately constant, we obtain $T_{\rm cl} \sim t^{-2/(1+2\beta)}$ and estimate the pressure in clusters, $P_{\rm cl} \sim f(n_{\rm cl})T_{\rm cl} \sim t^{-2/(1+2\beta)}$, where the factor f does not depend on T. The necessary condition for clusters to dissolve reads $P_{\rm cl} > P$ for $t \to \infty$; i.e., $\alpha + z > 2/(1 + 2\beta)$. With z given above this is equivalent to the condition $\beta > 1/2$; that is, gases only with a pronounced dependence of ε_T on T evolve to a uniform final state. In [10] a drastically simplified velocity-dependent coefficient of restitution was studied: $\varepsilon(g) = \text{const}$ if $g \geq g^*$ and $\varepsilon = 1$ if $g < g^*$ with g^* being a constant. For a gas of particles, interacting by this collision law (which qualitatively corresponds to $\beta \to \infty$), cluster formation is a transient phenomenon, although the temperature decays to zero [10]. For gases of viscoelastic particles $\beta = 1/10 < 1/2$; hence, it is not clear whether structures arise only temporarily in these systems or appear and get frozen.

To address this problem we study the evolution of a gas of viscoelastic particles by means of three independent methods: event-driven molecular dynamics (MD), numerical solution of the hydrodynamic (HD) equations, and linear stability analysis of the HD equations.

The MD simulations with periodic boundary conditions were performed for a 2D gas of $N = 10^5$ particles of diameter $\sigma = 1$, with the coefficient of restitution according to Eq. (1). The gas has the packing fraction $\phi = n\pi\sigma^2/4 = 0.2$, initial temperature $T_0 = 1$, and the dissipative coefficient $\gamma = 0.0577$ which corresponds to the initial coefficient of restitution $\varepsilon_T \sim 1 - \gamma \simeq 0.94$. Starting the simulations with homogeneous distribution of particles [homogeneous cooling state (HCS)], clusters appear and grow until they reach the *system size*; then they dissolve (Fig. 1). Figure 2 shows the evolution of the average particle energy, $E(t) = (1/2N)\sum_i m v_i^2$, which evolves in the HCS according to the modified Haff law [8],

$$E(t)/E_0 = T_{\rm h}(t)/T_0 = (1 + t/\tau_0)^{-5/3}, \qquad (2)$$

where

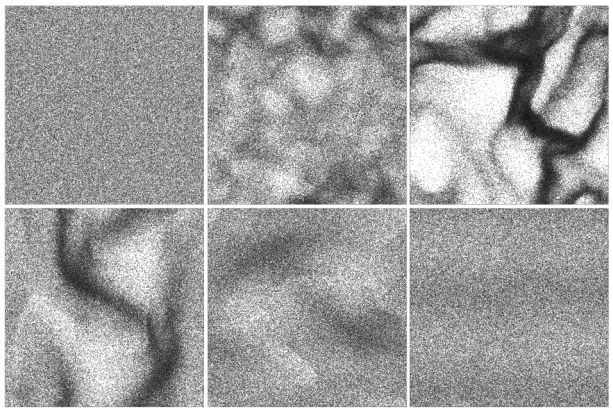

FIG. 1. MD simulation of $N = 10^5$ viscoelastic particles. Clusters appear as transient structures. The snapshots where taken after 0, 200, 800, 7500, 20 000, and 70 000 collisions per particle.

$$\tau_0^{-1} = (24/5) q_0 \tau_c^{-1}(0) \delta, \quad \delta = (\gamma/C_1)(T_0/m)^{1/10}. \tag{3}$$

Here $\tau_c^{-1}(t) = 2n\sigma g_2(\sigma)\sqrt{\pi T(t)/m}$ is the mean collision time, $g_2(\sigma) = (1 - 7\phi/16)/(1 - \phi)^2$ is the contact value of the pair correlation function. The constants $q_0 \approx 0.173$ and $C_1 \approx 1.1534$ are also known analytically [8]. At later times the deviation from the Haff law becomes pronounced; however, as the gas further evolves the clusters and vortices dissolve, and the system approaches the regime of homogeneous cooling; see Fig. 1. In the case of the above mentioned simplified model for $\varepsilon(g)$ [10], the temperature does not eventually return to the Haff law but decays logarithmically slow.

To explain the observed effects we consider the hydrodynamic equations [6,11,12] for the number density $n(\vec{r}, t)$, flow velocity $\vec{u}(\vec{r}, t)$, and temperature field $T(\vec{r}, t)$:

$$\frac{\partial n}{\partial t} = -\nabla_i (n u_i), \tag{4}$$

$$\frac{\partial u_i}{\partial t} = -(u_j \nabla_j) u_i + \frac{1}{nm} \nabla_j (\eta_{ijkl} \nabla_k u_l - P \delta_{ij}), \tag{5}$$

$$\frac{\partial T}{\partial t} = -(u_j \nabla_j) T - \frac{P}{n} (\nabla_i u_i) + \frac{1}{n} \eta_{ijkl} (\nabla_k u_l)(\nabla_j u_i) + \frac{1}{n} \nabla_i (\kappa \nabla_i T) + \frac{1}{n} \nabla_i (\mu \nabla_i n) - \zeta T. \tag{6}$$

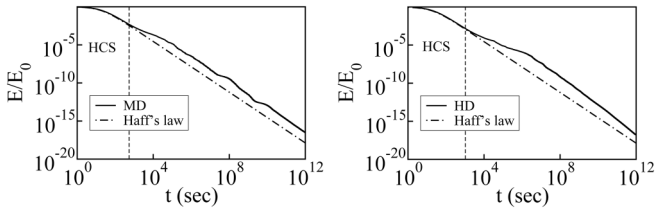

FIG. 2. The energy decay as obtained by MD (left) and by the numerical solution of the HD equations (right). The dash-dotted lines show the modified Haff law, Eq. (2). The end of the HCS is indicated by the vertical dashed lines.

Here $P = nT[1 + (1 + \varepsilon)\phi g_2(\sigma)]$ and $\eta_{ijkl} = \eta(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl})$ is the viscosity tensor. η and κ, respectively, are the coefficients of viscosity and thermal conductivity; ζ is the cooling coefficient and the coefficient μ is specific for granular gases [13,14]. The coefficients η, κ, μ, and ζ have been recently derived for a gas of viscoelastic particles [12]. They may be written as an expansion ($b = \eta, \kappa, \mu, \zeta$),

$$b = b_0 + b_1 \delta' + b_2 \delta'^2, \tag{7}$$

where $\delta'(t) = \delta[2T(t)/T_0]^{1/10}$ is the time-dependent dissipation parameter and the microscopic expressions for b_0, b_1, and b_2 are given in [12]. We stress that the temperature dependence of these coefficients differs drastically from the case $\varepsilon = \text{const}$; see, e.g., [13–15].

We numerically solve the hydrodynamic equations (4)–(6) with the coefficients Eq. (7) calculated for the same microscopic parameters γ, σ, and m as used for the MD simulations. We use a finite volume discretization scheme of global second order on a staggered grid. The integration in time is done through a transient variation diminishing multistep scheme of fourth order [16]. We use a 50×50 computational domain with periodic boundary conditions. Special care has been taken treating the advection terms in (4)–(6) [17].

We start the numerical integration with random initial conditions for the density and flow-velocity field (thermal fluctuations) and confirm the transient character of the pattern formation, Fig. 3. The cooling curve for $E(t)$ [18] demonstrates qualitatively the same behavior as observed in the MD simulations [Fig. 2 (right)]. To study the mechanism of pattern evolution more directly we considered initial conditions with a superimposed sinusoidal mode and observed similar transient structures. For rea-

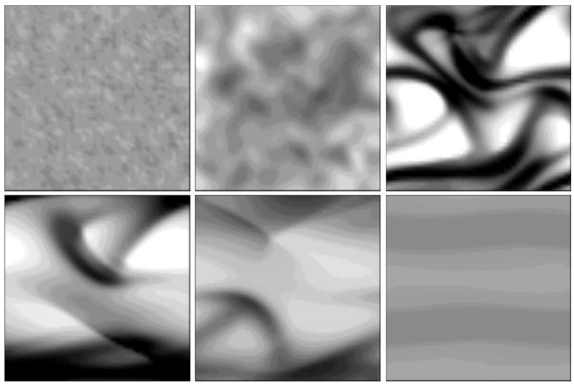

FIG. 3. The gas density obtained from the numerical solution of the HD equations (4)–(6) with periodic boundary and random initial conditions. The parameters γ, ϕ, T_0 are the same as in the MD simulations. Density inhomogeneities (clusters) appear but eventually dissolve. The snapshots were taken after 0, 200, 800, 7500, 20 000, and 70 000 collisions per particle, in correspondence to the snapshots in Fig. 1. The number of collisions was computed using the average temperature.

sons explained below, we have chosen the transverse velocity (shear) mode. It has the components $u_y(\vec{r},0) = u_{ky}(0)\sin(kx)$, $u_x(\vec{r},0) = 0$, $T(\vec{r},0) = T_0$, and $n(\vec{r},0) = n_h$, where $k = (2\pi/L)l$, $(l = 1, 2, \dots)$ is the wave number, L is the system size, and $u_{ky}(0)$ is the initial amplitude of the mode. Solving the hydrodynamic equations numerically we analyze the evolution of the shear mode, Fig. 4, the longitudinal mode, and the density mode, Fig. 5. As it follows from Fig. 4, the shear mode (in reduced units) is unstable for wave vectors smaller than a threshold value. This instability leads to the formation of vortices [3,4]. The growing shear mode initiates the growth of the mode of longitudinal velocity which, in its turn, causes a growth of the density mode corresponding to clustering; see Fig. 5. This indicates that clustering is driven mainly by a nonlinear mechanism [1,4]: As explained below, a single *transverse* mode cannot excite by a linear mechanism, neither a longitudinal mode, nor a density mode. Hence only nonlinear coupling between the shear and longitudinal modes may cause the observed excitation of the longitudinal mode [19], which further initiates the growth of the density mode, i.e., clustering. Similar mechanisms are responsible for pattern formation in a gas with $\varepsilon = \text{const}$ [1,4]. Contrary to the case $\varepsilon = \text{const}$, in a force-free gas of viscoelastic particles all modes eventually decay, and only transient structures appear.

To obtain quantitative estimates we perform a stability analysis of the HD equations (4)–(6) with respect to the HCS at density n_h, and temperature $T_h(t)$. We assume that the deviations $\delta T(\vec{r},t) = T(\vec{r},t) - T_h(t)$ and $\delta n(\vec{r},t) = n(\vec{r},t) - n_h$ are small,

$$\theta \equiv \frac{\delta T}{T_h} \ll 1, \quad \rho \equiv \frac{\delta n}{n_h} \ll 1, \quad |\vec{w}| \equiv \frac{|\vec{u}|}{v_T} \ll 1 \qquad (8)$$

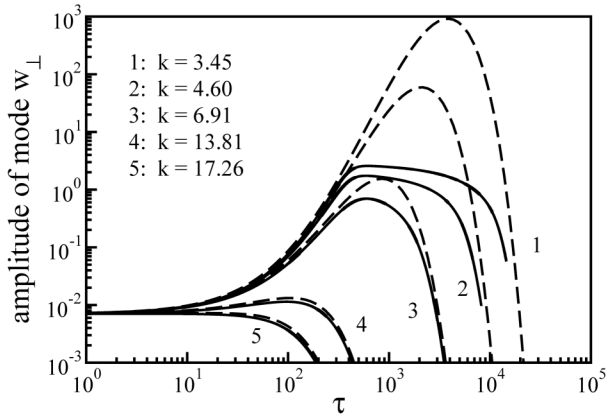

FIG. 4. Evolution of the reduced amplitude of the shear mode, $w_{k,\perp}(\tau) \equiv u_{ky}(\tau)/v_T(\tau)$. Initially only a single shear mode with $k = 2\pi/L$ and with an amplitude of the order of the thermal fluctuations is excited. Full lines: numerical solution of the hydrodynamic equations; dashed lines: results of the linear analysis, Eq. (14). The parameters are the same as in Fig. 3. Dimensionless time and length are used (see the text). Note that the different k correspond to a different system size.

and linearize these equations. Below we use the dimensionless time τ, measured in units of $\tau_c(t)/2$, and dimensionless length $\vec{r}$, measured in units of $l_0/2$ ($l_0^{-1} = \sqrt{2\pi}n\sigma g_2(\sigma)$ is the mean free path) and write the linearized equations for the Fourier transforms of the fields $\theta(\vec{r},t)$, $\rho(\vec{r})$ and $\vec{w}(\vec{r},t)$:

$$\frac{\partial \vec{w}_{\vec{k}\perp}}{\partial \tau} = [\beta\delta'(\tau) - k^2]\vec{w}_{\vec{k}\perp}, \qquad (9)$$

$$\frac{\partial \rho_{\vec{k}}}{\partial \tau} = -ikw_{\vec{k}||}, \qquad (10)$$

$$\frac{\partial \theta_{\vec{k}}}{\partial \tau} = -[4\tilde{\mu}_1 k^2 + 2\beta]\delta'(\tau)\rho_{\vec{k}} - [4k^2 + (6\beta/5)\delta'(\tau)]\theta_{\vec{k}} - ikw_{\vec{k}||}, \qquad (11)$$

$$\frac{\partial w_{\vec{k}||}}{\partial \tau} = -\frac{1}{2}ik\rho_{\vec{k}} - \frac{1}{2}ik\theta_{\vec{k}} + [\beta\delta'(\tau) - k^2]w_{\vec{k}||}. \qquad (12)$$

Here $w_{\vec{k}||}$ and $\vec{w}_{\vec{k}\perp}$ are, respectively, the longitudinal (i.e., parallel to the wave vector $\vec{k}$) and transversal (i.e., perpendicular to $\vec{k}$) components of the Fourier mode $\vec{w}_{\vec{k}}(t)$, $\beta = 2^{9/10}q_0 \approx 0.323$ and $\tilde{\mu}_1 = 1.811$ are the constants. To obtain Eqs. (9)–(12) we keep only leading-order terms with respect to the dissipative parameter $\delta'(t)$ in the expansion Eq. (7) for the coefficients η, κ, μ, ζ [12]. Note the important difference between the linearized equations (9)–(12) and the corresponding equations for the case $\varepsilon = \text{const}$: In the latter case the coefficients in these equations are constant (e.g., [4,5]), while in the former case they depend on time via

$$\delta'(\tau) = 2^{1/10}\delta[1 + 2q_0\delta\tau/5]^{-1}. \qquad (13)$$

The solution for $\vec{w}_{\vec{k}\perp}(\tau)$ reads

$$\vec{w}_{\vec{k}\perp}(\tau) = \vec{w}_{\vec{k}\perp}(0)[1 + 2q_0\delta\tau/5]^5 e^{-k^2\tau}, \qquad (14)$$

where $\vec{w}_{\vec{k}\perp}(0)$ is the initial amplitude of the shear mode. There exists a critical wave number $k_\perp^* \equiv \sqrt{2q_0\delta}$, which separates two regimes: Shear modes with $k \geq k_\perp^*$ always decay, while those with $k < k_\perp^*$ initially grow and reach a

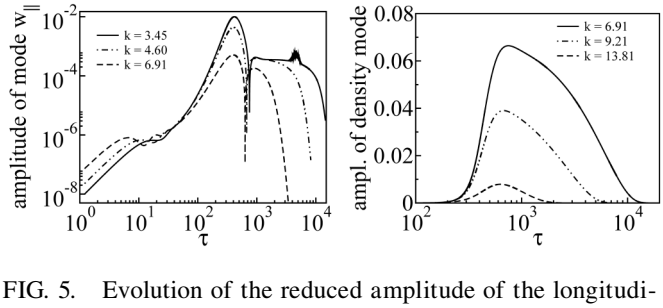

FIG. 5. Evolution of the reduced amplitude of the longitudinal mode, $w_{k,\|}(\tau) \equiv u_{kx}(\tau)/v_T(\tau)$ (left) and of the density mode $\rho_k(\tau)$ (right). Parameters, units, and initial conditions are the same as in Fig. 4.

maximum,

$$w_{\vec{k}\perp}^{\max} = w_{\vec{k}\perp}(0)\left[\frac{2q_0\delta}{k^2 e}\right]^5 \exp\left(\frac{5k^2}{2q_0\delta}\right) \qquad (15)$$

at $\tau_{k\perp}^* = 5/k^2 - 5/(2q_0\delta)$; then they decay and die off completely. The formation of vortices is attributed to the growth of the shear mode $\vec{w}_{\vec{k}\perp}$ [4,5]; therefore, the vortices of size $\sim k^{-1}$ decay after a transient time $\sim\tau_{k\perp}^*$. Any system of size $\sim L$ has a minimal wave number $\sim 2\pi/L$; hence *all* shear modes decay by the time $\tau_\perp^* \sim 5L^2/4\pi^2 - 5/(2q_0\delta)$.

To perform the stability analysis for the other three modes we write Eqs. (10)–(12) in the form

$$\dot{\mathbf{\Psi}}_k = \hat{\mathbf{M}}_k(\tau)\mathbf{\Psi}_k, \qquad \mathbf{\Psi}_k \equiv (\rho_{\vec{k}}, \theta_{\vec{k}}, w_{\vec{k}\|})^T. \qquad (16)$$

The matrix $\hat{\mathbf{M}}_k(\tau)$ has *time-dependent* eigenvalues and eigenmodes, which for small dissipation δ are analogous to the sound and the heat mode of a gas with a constant ε [4,5]. For large wave numbers k all the modes decay, while for small k the heat mode may grow. The critical k may be found from the condition $\dot{\mathbf{\Psi}}_k = 0$, or $\det|\hat{\mathbf{M}}_k(\tau)| = 0$:

$$k_\|^*(\tau) \simeq \frac{1}{4\sqrt{5}}(2^{1/10}\beta\delta)^{1/2}\left[1 + \frac{2}{5}q_0\delta\tau\right]^{-1/2}. \qquad (17)$$

Modes with $k > k_\|^*(0)$ always decay, while those with $k < k_\|^*(0)$ may initially grow. Since $k_\|^*(\tau)$ decreases with time even a mode with $k < k_\|^*(0)$, which initially grows, starts to decay after a transient time, when the condition $k > k_\|^*(\tau)$ is fulfilled.

The value of $k_\|^*(\tau)$ becomes smaller than the minimal wave number $2\pi/L$ at time $\tau_\|^* \sim L^2/16 - 5/(2q_0\delta)$; i.e., for $\tau > \tau_\|^*$ the amplitude of any of the modes $\rho_{\vec{k}}$, $\theta_{\vec{k}}$, $w_{\vec{k}\|}$ decays. Note that $\tau_\perp^* > \tau_\|^*$ in agreement with the simulation results (Figs. 4 and 5). Since clustering and vortex formation is attributed to the instability of the heat and shear modes [1,3,14] we conclude that the eventual decay of all modes predicted by the linear stability analysis implies the transient structure formation.

We have studied a force-free granular gas of viscoelastic particles by means of MD, a numerical solution of the HD equations, and a linear stability analysis of the HD equations. All three methods indicate that structure formation in a gas of viscoelastic particles occurs only as a transient phenomenon, whose duration increases with the system size N for the same particle number density. Correspondingly, for larger N the structures appear to be denser and more long-lived, whereas an extrapolation to the unbounded system cannot be easily concluded from these arguments. The finite duration of the cluster phase is in sharp contrast to the case of a gas with a simplified collision model $\varepsilon = \text{const}$, where structures have been proven to arise and to continuously develop. In our simulations, due to the limited system size and periodic boundary conditions, we have unphysical self-interactions of the clusters. We believe, however, that this effect does not invalidate the main conclusion of our study of the transient character of structure formation in force-free granular gases. This expectation is also supported by MD simulations using the simplified model $\varepsilon(g)$ given in [10] which has the same limit as Eq. (1), $\varepsilon(g = 0) = 1$: Here the clusters arise and grow; however, they decay before growing to system size [10].

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[17] B. P. Leonard, Comput. Methods Appl. Mech. Eng. **88**, 17 (1991). For small systems one can use a simple QUICK scheme. In bigger systems very dense transient clusters with a sharp boundary appear and "shock capturing" schemes or limiters must be used. We use a third order upwinding scheme (QUICKEST) with a limiter.
[18] In the hydrodynamic description the total energy $E(t)$ contains the thermal energy $n(\vec{r}, t)T(\vec{r}, t)$ and the energy of the fluxes $(m/2)n(\vec{r}, t)\vec{u}^2(\vec{r}, t)$ [3].
[19] For $w_{k,\|}(t)$ we observed a second peak, Fig. 5. Presently, it is not clear, whether it is attributed only to nonlinear effects or to the periodic boundary conditions, too.