Length Scales of Clustering in Granular Gases

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Clustering of granular gases is caused by the dissipation occurring in particle collisions. We use the generalized dimension, a measure for the inhomogeneity of a spatial distribution of particles to characterize the structural evolution. Furthermore, we quantify the typical length scale of the clusters obtained by 3D simulations using the index of dispersion, a measure for the deviation of the particle density from a Poissonian. We then derive an expression for the expected length scales of cluster formation from a stability analysis in the hydrodynamical approximation. We find a good agreement between our theoretical prediction and numerical experiments. [S0031-9007(99)09344-8]

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In recent studies much attention has been devoted to the dynamics of granular gases [1–8]. The difference of such systems to conventional gases is the energy loss occurring in interparticle collisions, characterized by the coefficient of restitution ϵ, the ratio between the normal components of the rebound velocity, and the impact velocity of the colliding particles. The dissipation leads to several phenomena that show a completely different behavior than conventional gases, e.g., permanent cooling of the gas in the absence of energy sources, clustering of the particles with continued cooling [1], or a nonequipartition of the translational and the rotational degrees of freedom [2]. Therefore, the study of granular gases represents an extension of the Boltzmann theory of classical gases.

In this Letter, we present a method of cluster detection of nearly homogeneous distributed assemblies in 3D and then compare this with a quantitative expression of the cluster sizes derived from stability analyses in the hydrodynamic approach. Namely, we characterize and quantify the clustering of granular assemblies through a statistical analysis of the phase-space data obtained from particle simulations. We introduce two statistical measures to accomplish that:

(i) To characterize the increase of clustering in the particle density with time, we define a quantity in terms of the generalized dimensions, a measure for the inhomogeneity of a spatial distribution of particles [9]. This quantity reflects the ϵ dependence of clustering formation. We find a monotonic dependence of the rate of clustering on the dissipation.

(ii) To quantify the characteristic size of inhomogeneities, we define another quantity in terms of the index of dispersion [10], which is a measure for the deviation of the particle density from a Poissonian. We find that the dependence of cluster size on ϵ, as obtained from our 3D simulations, agrees well with our theoretical predictions derived from a stability analysis using a hydrodynamical approximation [e.g., Eq. (6)]. Numerical simulations have shown [3] that the beginning of the cooling process is well described by the *homogeneous cooling state* (HCS), while, after a certain critical time, depending on the number of collisions per particle C/N, the cooling process is slowed down by velocity and density fluctuations. After this critical moment, the cooling is almost no longer determined by particle-particle but by cluster-cluster interactions. This would imply that the clusters have already been formed during this HCS phase.

In our simulations, we use a 3D event-driven code with $N \approx 50\,000$ identical spherical particles. The particle ensemble is simulated in a cubic box of side length $L_{\mathrm{box}} \approx 220$ particle radii, chosen to correspond to a filling factor of about 0.02. We use periodic boundary conditions where we prevent overlapping by creating a twin particle of every particle reaching the boundaries. The twin particles are shifted by an amount of $2L_{\mathrm{box}}$ to the opposite boundary and they get the same velocities and coordinates as the original particles. The original particles are removed from the system when the twin particle is completely inside the simulation box again. A particle leaving the box at the edge or the corners needs, of course, four or eight twins, respectively. Initially each particle is placed randomly in the box, checked for overlaps with already placed particles, and regenerated if an overlap occurs. Then each particle gets a velocity of a given absolute value with a randomly chosen direction.

In our simulations only translational degrees of freedom are considered. For convenience, we restrict ourselves to the case of constant coefficients of restitution and fix its values at $0.1, 0.2, \ldots, 1.0$. In recent studies we have shown that a variable coefficient of restitution slows down the process of cluster formation but does not prevent clustering at all, i.e., the HCS is elongated [4].

The inelastic collapse that has been found in 1D and 2D and could be expected in 3D [5] is due to the low filling factor not detected in our runs. However, it cannot be expected if one considers a finite contact duration [6].

We simulate the assemblies of different ϵ for the same ratio of collisions per particle $C/N \approx 12$. We ensure to be in the HCS phase by comparing the temperature evolution of the granular assembly measured by the numerical experiment with theoretical expressions derived from the

Boltzmann theory [1,7,8]. A deviation of the theory and the numerical simulation indicates an abandonment of the HCS phase.

In a granular system which is still in the HCS, inhomogeneities are difficult to distinguish from fluctuations of an ensemble with purely elastic particle interactions. Therefore, we use measures from nonlinear dynamics and statistics to characterize and quantify the spatial inhomogeneities in our simulations. First, we split the box into $m = 2^{\mathcal{L}}$ sub-boxes, where $\mathcal{L} = 1, 2, \ldots, 12$. Note that the sub-boxes are no cubes in general. Second, we characterize the cluster formation quantitatively, using the generalized dimension, based on the Rényi entropies [11] defined as $H^{(q)} = [1/(1-q)] \log \sum_{l=1}^{m} p_l^q$ with $q \in \mathbb{R} \setminus \{1\}$ and the probability p_l for particles to be in the lth box labeled by $m = 2^{\mathcal{L}}$.

Recently, we have shown that the generalized dimension D_q, defined in terms of $H^{(q)}$, is an appropriate tool to characterize the time evolution of the degree of clustering [9,12]. It is defined by $D_q = -\lim_{d\to 0} H^{(q)}/\log d$ for each time step t and restitution coefficient ϵ, where d is the diagonal of each sub-box. As q increases from 1, D_q accentuates more and more the degree of clumping (high density regions) while, as q decreases from 1, D_q accentuates better the degree of depletion (low density regions). To characterize the increase of inhomogeneity with time, we calculate from the simulation data how D_q changes with q, i.e., $\partial D_q(\epsilon, t)/\partial q$. Then, to get a representative measure of the change of inhomogeneity with time, we introduce the quantity (for $q \to 0$)

$$\Lambda(\epsilon) = \frac{\partial D_q(\epsilon, t = t_0)/\partial q}{\partial D_q(\epsilon, t = t_{\max})/\partial q}, \tag{1}$$

where t_0 and $t_{\max}$ are the times at the beginning and at the end of the simulation, respectively. The value Λ, based on the change of the generalized dimension with q reflects the ϵ-dependent structure formation. This measure is more detailed and therefore more suitable for 3D simulations than the measure $H^{(q)}$ with $q =$ const used in [4]. As well, the quantity Λ is more sensitive for detecting density inhomogeneities in our runs than the well-known two-point correlation function. Figure 1 shows the dependence of Λ on ϵ indicating that an initially homogeneous distribution of particles changes the greatest the smaller the coefficient of restitution ϵ is. For elastically colliding granules ($\epsilon = 1$), one gets $\Lambda = 1$ corresponding to an unchanged homogeneous particle distribution during the time evolution. This behavior agrees with predictions [1,4] that, as the dissipation per collision $(1 - \epsilon^2)$ increases, the clustering becomes more intense.

However, it is not possible to quantify, using this method, the length scales of the inhomogeneities in the particle density of the simulations. Therefore, we introduce a new measure defined in terms of the index of dispersion [10]. The test statistic of the index of dispersion is given by $I = (m-1)s^2(n)/\langle n \rangle_l$ with the particle density $n = n(\epsilon, l, d, t)$ in the lth box, the standard deviation $s^2 = \sum_{l=1}^{m}(n - \langle n \rangle)^2/(m-1)$, and the number of degrees of freedom m (total number of boxes). This test statistic is that of a χ^2 goodness-of-fit test for the hypothesis that the particles are independently and uniformly distributed in the whole simulation box.

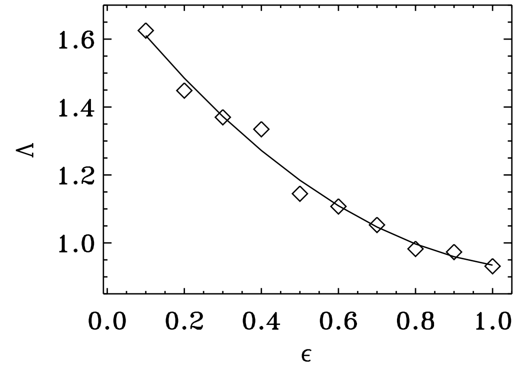

FIG. 1. Λ vs ϵ [Eq. (1)]. The diamonds are the data points; the solid line is the result of a quadratic regression fit.

For a homogeneous particle distribution, the index of dispersion satisfies $\chi^2_{m-1,1-\alpha} < I < \chi^2_{m-1,\alpha}$, which is characteristic for a Poissonian distribution of particles. Here, α is the significance level of the χ^2 statistics. A higher index of dispersion $I > \chi^2_{m-1,\alpha}$ points towards inhomogeneities, while $I < \chi^2_{m-1,1-\alpha}$ is typical for a regular distribution of particles, as it is found, e.g., in lattices. To detect the inhomogeneities, we define the normalized quantity

$$\tilde{I} = \left[\frac{I}{\chi^2_{m-1,\alpha}} - 1\right] \Theta_H\left(\frac{I}{\chi^2_{m-1,\alpha}} - 1\right), \tag{2}$$

where we relate the index of dispersion to the critical value $\chi^2_{m-1,\alpha}$. We checked different significance levels of the χ^2 statistics, namely, $0.01 \le \alpha \le 0.07$, which show similar results. Figure 2 and the following calculations are done with $\alpha = 0.05$. The Heaviside function Θ_H ensures that purely regular features are excluded from the statistical treatment. The time evolution of $\tilde{I}$ in the critical region ($I > \chi^2_{m-1,\alpha}$) for different values of ϵ, obtained from the 3D simulations, is shown in Fig. 2. The clumping starts at the smallest scales after a characteristic time. At later times, inhomogeneities at larger scales evolve. Figure 2 shows the tendency of the values $\tilde{I}$ as a function of L, ϵ and time. Because of the finite number of particles used in the simulations, one observes, in addition to the density inhomogeneities caused by the dissipation, fluctuations $\propto 1/\sqrt{N}$. The most prominent length scale of the inhomogeneities, under these conditions, is obtained as follows. From our simulations and analysis, we find the following expression for the critical length scale L_c by averaging the sub-box diagonal d over space and time, as

$$L_c(\epsilon) = \frac{\sum_d d \sum_{C/N} \tilde{I}}{\sum_d \sum_{C/N} \tilde{I}}. \tag{3}$$

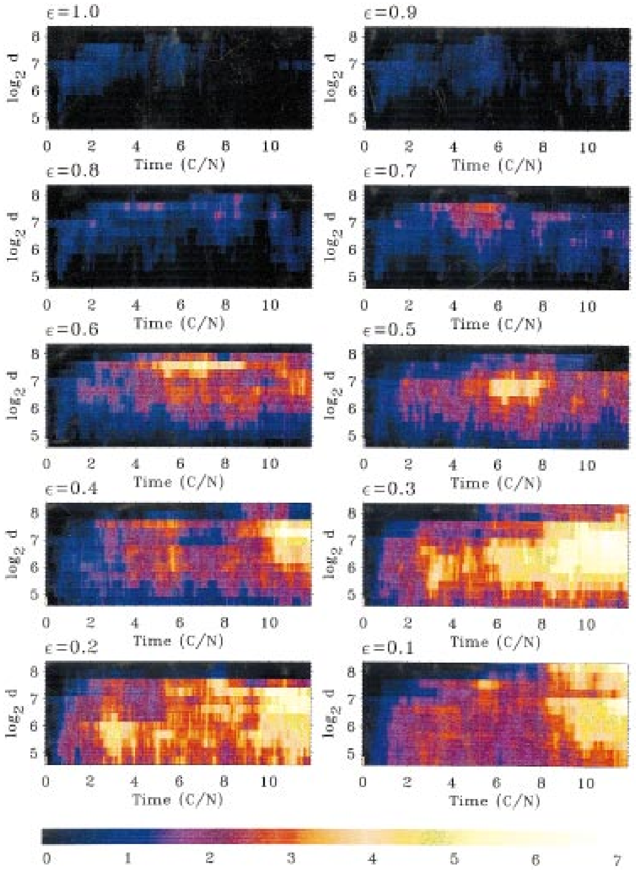

FIG. 2(color). The evolution of the index of dispersion [Eq. (2)] in the critical region $\tilde{I}$ vs the sub-box diagonal d and the number of collisions per particle C/N for different restitution coefficients ϵ. The value of $\tilde{I}$ is color coded as indicated in the color bar. Black indicates a Poissonian distribution ($\tilde{I} = 0$); values higher than 0 (colored) indicate a significant lumpy distribution of the particles in the configuration space. White corresponds to the highest deviation from a Poissonian particle distribution.

To interpret and better understand the results of our simulations, we use a stability analysis in the hydrodynamical approximation, which describes well the physics of a granular gas during the HCS phase [1,3,4,7]. The equations of hydrodynamics for a force-free granular gas read as

$$\frac{d\rho}{dt} = -\rho\nabla\cdot\vec{u}, \qquad \rho\frac{d\vec{u}}{dt} = -\nabla\cdot\hat{P},$$
$$\text{and} \qquad \frac{3}{2}\rho\frac{dT}{dt} = -\nabla\cdot\vec{Q} - \hat{P}:\nabla\circ\vec{u} - \gamma, \tag{4}$$

where the material derivative is given by $d/dt \rightarrow \partial/\partial t + \vec{u}\cdot\nabla$; ":" and "$\circ$" denote the double inner product and the dyadic product, respectively. The quantities ρ, $\vec{u}$, and T are the density, the average particle velocity, and the temperature, respectively. The heat flux is $\vec{Q} = -\kappa\nabla T$, and the pressure tensor is denoted by $\hat{P}(\hat{D}) = p\hat{\mathbf{I}} - 2\eta\hat{D}$ with the shear tensor $\hat{D} = \frac{1}{2}(\nabla\circ\vec{u} + \vec{u}\circ\nabla)$, where p is the pressure and $\hat{\mathbf{I}}$ is the unity tensor. The constitutive relations in the dilute limit read for a constant coefficient of restitution [7] $\eta = 5\sqrt{T}/4\sigma^2\sqrt{\pi}(3-\epsilon)(1+\epsilon)$ for the viscosity, $\kappa = 75\sqrt{T}/2\sigma^2\sqrt{\pi}(1+\epsilon)(49-33\epsilon)$ for the heat conductivity, and $\gamma = 2\rho^2\sigma^2\sqrt{\pi T^3}(1-\epsilon^2)$ for the cooling. Here, the mass and the Boltzmann constant are $m = k_B = 1$ and σ is the particle diameter.

In order to analyze the stability of an initially homogeneous granular gas, we linearize the hydrodynamic Eq. (4) and expand the state variables about the ground state $\vec{X} = \vec{X}_0(t) + \vec{X}'(\vec{r},t)$ with $|\vec{X}'/\vec{X}_0| \ll 1$. For a force-free granular gas, ρ_0 is constant in time and space, $\vec{u}_0 = 0$, and the ground state temperature T_0 is a function of time, due to the permanent cooling. In a periodic or infinite system, the eigenfunctions of the linearized Eq. (4) are plane waves $\vec{X}'(\vec{r},t) \propto \exp(\alpha t + i\vec{k}\cdot\vec{r})$, where $\vec{k}$ is the wave vector and α is the growth rate. Without loss of generality, one can choose $\vec{k} = (k,0,0)$. The resulting eigenvalue problem gives a system of linear equations $\{\hat{\mathbf{A}} - \alpha\hat{\mathbf{I}}\}\vec{X}' = \vec{0}$, where $\hat{\mathbf{A}}$ is the coefficient matrix with the characteristic equation $|\hat{\mathbf{A}} - \alpha\hat{\mathbf{I}}| = 0$, determining a characteristic third order polynomial. If one of its roots takes $\mathrm{Re}(\alpha) > 0$, an instability is found. The linear stability analysis yields a condition, for which an initially homogeneous granular ensemble becomes monotonically unstable [4],

$$\frac{\gamma_0}{\rho_0}\frac{\partial p}{\partial T}\bigg|_0 - \frac{\partial\gamma}{\partial\rho}\bigg|_0\frac{\partial p}{\partial T}\bigg|_0 + \frac{\partial\gamma}{\partial T}\bigg|_0\frac{\partial p}{\partial\rho}\bigg|_0 + \kappa_0\frac{\partial p}{\partial\rho}\bigg|_0 k^2 < 0\,. \tag{5}$$

The subscript 0 denotes the ground state about which the linear stability analysis is carried out. To quantify the derivatives in Eq. (5), we apply the equation of state of an ideal gas with ρ as an independent variable $p = \rho T(\rho)$. Using this, we get $\partial p/\partial T|_0 = \rho_0$, $\partial p/\partial\rho|_0 = T_0 + \rho_0\partial T/\partial\rho|_0$, $\partial\gamma/\partial T|_0 = 3\gamma_0/2T_0$, and $\partial\gamma/\partial\rho|_0 = 2\gamma_0/\rho_0 + 3\gamma_0/2T_0\cdot\partial T/\partial\rho|_0$. This yields an expression for the critical wave number $k_c = \sqrt{-\gamma_0/2\kappa_0\partial p/\partial\rho|_0}$. According to this equation, unstable wavelike oscillations with a characteristic length scale $L_c = 2\pi k_c^{-1}$ occur only if $\partial p/\partial\rho|_0 < 0$, which quantifies the pressure instability mentioned above.

The number of collisions per particle as a function of the "real" time is given by $C/N = \frac{1}{2}\int_0^t \bar{v}/\lambda\, dt'$ with the average velocity $\bar{v} = \sqrt{8T/\pi}$ and the mean free path $\lambda = (\sqrt{2}\pi\sigma^2\rho)^{-1}$. In the dilute limit, the temperature evolution of an initial homogeneous granular gas with $\epsilon =$ const and an initial temperature T_{in} is given by $T(t) = T_{\mathrm{in}}/(1 + t/t^*)^2$ with $t^* = [\frac{2}{3}(1-\epsilon^2)\rho\sigma^2\sqrt{\pi T_{\mathrm{in}}}]^{-1}$. Using this, one finds $C/N = 3/(1-\epsilon^2)\ln(1 + t/t^*)$. The temperature in terms of C/N is then given by $T(\frac{C}{N}) = T_{\mathrm{in}}\exp(-2\frac{C}{N}\frac{(1-\epsilon^2)}{3})$, and $\partial p/\partial\rho|_0 = T_0[2\exp(-\frac{C}{N}\times\frac{(1-\epsilon^2)}{3}) - 1]$ which, together with the constitutive relations for κ and γ yields the critical wave number

$$k_c = \sqrt{-\frac{\gamma_0}{2\kappa_0 T_0}\left[2\exp\left(-\frac{C}{N}\frac{(1-\epsilon^2)}{3}\right)-1\right]^{-1}}\,. \tag{6}$$

Because of the ϵ dependence of γ_0 there is no clustering for $\epsilon = 1$. Especially, for $C/N \to \infty$ ($\epsilon \neq 1$) one gets $k_c \propto \sqrt{1-\epsilon^2}$, which is the result found by Goldhirsch and Zanetti [1], where the derivative $\partial p/\partial \rho$ has been assumed to be a negative constant (the ϵ dependence of κ_0 has only little influence on the shape of k_c). In Fig. 3, the wave number k_c derived from numerical simulations is compared with the corresponding theoretical relation for k_c [Eq. (6)] as a function of ϵ and $C/N \to \infty$ (dotted line). Note that the stability analysis yields a k_c corresponding to a "full" wavelength, while the critical length scale given by Eq. (3) corresponds to the detection of inhomogeneities according to the size of the chosen sub-box. Therefore, to compare the results of the simulations with the theoretical investigations, we have to multiply the measured L_c by a factor of 2. We find a fairly good agreement between the theoretical approach and the numerical experiments. This confirms the validity of the theory to explain cluster formation, including the major quantitative property such as the typical cluster size. The rather small deviation of the theoretical curve from the data points is due to fluctuations associated with the finite number of particles and the averaging procedure. The dotted line corresponds to the wave number k_c of the homogeneous cooling for $C/N \to \infty$, indicating that no dramatic change of cluster formation can be expected under homogeneous cooling state conditions. For $\epsilon = 1$, where one expects $k_c = 0$, fluctuations on all scales yield length scales in the range of half of the box size Eq. (3), while for $\epsilon < 1$, Fig. 3 shows a systematic dependence on the dissipation.

To judge whether there is an influence of the box size on our measurements, we vary the number of particles and adequate the box size at a filling factor of 0.02 for $\epsilon = 0.4$. In Fig. 3 the result for $N \approx 40\,000$ and $N \approx 100\,000$ is shown, indicating that there is no systematic dependence on the box sizes.

In conclusion, our theoretical investigations, based on a stability analysis of the hydrodynamical equations, Eq. (4), yield typical cluster sizes depending on the dissipation, represented by the wave number k_c [Eq. (6)]. Using the generalized dimension we characterize the structural evolution of density inhomogeneities. Statistical analyses of 3D numerical simulation data, based on the index of dispersion, yield typical length scales of cluster formation [Eq. (3)] as a function of the restitution ϵ, which is in good agreement with our theoretical predictions [Eq. (6)]. Both the theoretical investigations as well as the computer simulations are restricted to the HCS. An analysis of the cooling regime beyond the homogeneous cooling state is needed and is part of ongoing and future work.

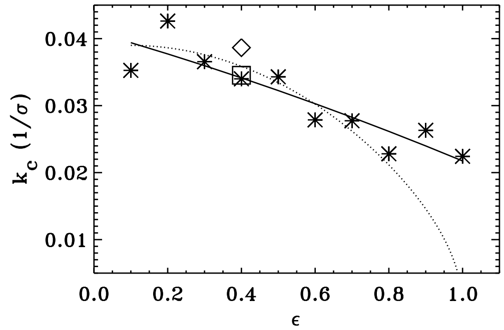

FIG. 3. Critical wave number k_c vs ϵ. The stars are the data points obtained from the simulations, the solid line shows the curve for the quadratic regression fit. The dotted line is the theoretical result for $C/N \to \infty$. Diamonds and squares are the results for $N \approx 40\,000$ and $100\,000$, respectively. To get the length scales of the measured inhomogeneities, the corresponding k_c has to be divided by 2.

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