

Ordering Phenomena in Cooling Granular Mixtures

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We report two phenomena, induced by dynamical correlations, that occur during the free cooling of a two-dimensional mixture of inelastic hard disks. First, we show that, due to the onset of velocity correlations, the ratio of the kinetic energies associated with the two species changes from the value corresponding to the homogeneous cooling state to a value approximately given by the mass ratio m_1/m_2 of the two species. Second, we report a novel segregation effect that occurs in the late stage of cooling, where interconnected domains appear. Spectral analysis of the composition field reveals the emergence of a growing characteristic length.

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A gas of inelastic hard spheres (IHS), due to its relative simplicity, represents a standard reference model for fluidized granular materials [1]. Many of its properties are well understood. In particular, a great deal of attention has been devoted to the study of the cooling process that occurs when an assembly of grains, initially in motion, evolves in the absence of any external energy feed. In this case, while the asymptotic state (all particles at rest) is trivial, the dynamics of the cooling process displays several interesting features. Three stages can be identified:

(i) After an initial transient, during which the velocity distribution is not necessarily Maxwellian [2], the system enters the homogeneous cooling state (HCS), where the average kinetic energy decreases according to Haff's law [3], $K(t) = K(0)/(1 + t/t_0)^2$. Such a state is characterized by a uniform density and a lack of strong correlations among the velocities [4].

(ii) An intermediate regime, wherein the system remains homogeneous, but the velocity field develops vortices (Fig. 1). These vortices result from the parallelization of velocities induced by inelasticity. Because of the progressive buildup of velocity correlations, the kinetic energy decays as $t^{-d/2}$ [5–7].

(iii) Goldhirsch and Zanetti [5] suggested that vortices represent the physical mechanism leading to the third stage, wherein the density field itself loses its homogeneity and dense clusters appear, surrounded by rarefied regions. At this stage neither the velocity nor the temperature fields are homogeneous anymore (see Fig. 1).

Most of the existing information on the cooling properties of granular matter concern one-component systems. A few investigations on binary mixtures [8,9] focused on the HCS only. Garzó and Dufty [8] showed that for a binary mixture the average kinetic energies per particle—i.e., the kinetic temperatures K_1 and K_2 of the two species—are different, and their ratio $\gamma = K_1/K_2$ remains constant in the HCS.

In this Letter we explore the cooling dynamics of a mixture of inelastic hard disks across the previously listed dynamical regimes by using an event-driven molecular dynamics simulation and a recently introduced lattice model [10]. We show that during the second stage of cooling—at the onset of local velocity correlations—the ratio of the kinetic temperatures of the two species sharply departs from the nearly steady value attained during the homogeneous cooling stage, and eventually

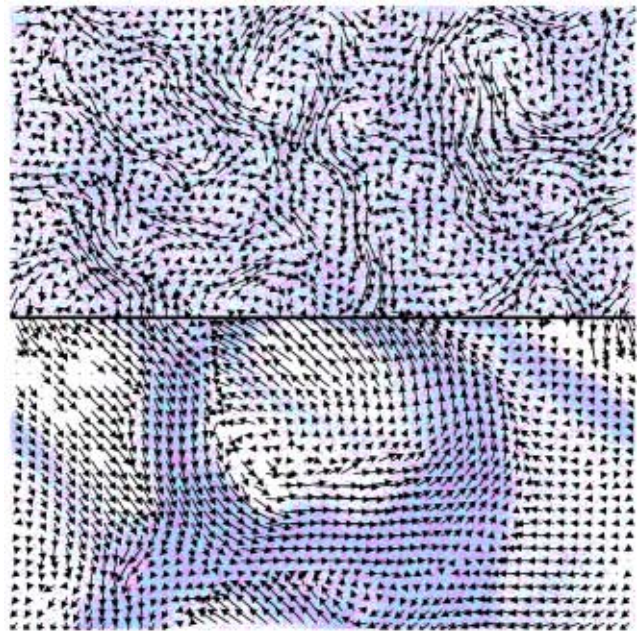


FIG. 1 (color online). Status of the system at points A (upper panel) and B (lower panel) of Fig. 2. The instantaneous velocity field is superimposed. Early vortices can be seen in the upper panel, with particles still (approximately) uniformly distributed. In the lower panel, dense clustering has appeared and the typical size of vortices has significantly increased. Strong correlations in the velocity field are visible.

approaches an asymptotic value that depends only on the mass ratio of the two species. In the last stage we find evidence for segregation of the species, which is revealed both by local indicators and by spectral analysis of the composition field.

For our model we consider a two-dimensional (2D) system containing $N_1 = 5 \times 10^4$ and $N_2 = N_1$ disks of equal radius R and masses m_1 and m_2 , respectively. Initially, the disks are uniformly distributed in a square domain of side $L = 10^3 R$, with periodic boundary conditions, and their velocities are set by sampling Maxwell distributions corresponding to the same temperature. In the IHS model the collisions are instantaneous, conserve total momentum, and dissipate a fraction of the kinetic energy. The velocity \mathbf{v}'_j of a particle j after collision is

$$\mathbf{v}'_j = \mathbf{v}_j + \mu_{ij}[1 + r(v_n)]v_n \mathbf{n}, \quad (1)$$

where $\mathbf{n} = (\mathbf{r}_i - \mathbf{r}_j)/|\mathbf{r}_i - \mathbf{r}_j|$ is the unit vector joining the centers \mathbf{r}_i and \mathbf{r}_j of the disks at contact, $v_n = (\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{n}$ is the relative normal velocity of the disks before collision, $\mu_{ij} = m_i/(m_i + m_j)$, and $r(v_n)$ is a velocity-dependent coefficient of restitution. Inelastic collapse is avoided by choosing a $r(v_n)$ such that, for relative normal velocities falling below a threshold v_0 , r approaches unity when $v_n \rightarrow 0$, according to the power law given in Ref. [11]. Different cutoff velocities were simulated in order to ascertain the robustness of the investigated properties. An efficient event-driven simulation allowed us to probe the late stages of the cooling process [12].

During the initial homogeneous cooling phase, the behavior of the mixture is well described by the Boltzmann-Enskog (BE) transport equation [8]. Theoretical values for the ratio γ can be computed within this framework, and their values for the chosen set of microscopic parameters are shown in Fig. 2 (dashed lines). These theoretical values agree with the initial plateau observed in the temporal evolution of γ . However, since the BE approach, by construction, neglects velocity correlations, one can expect that the intermediate cooling regime cannot be properly described within its framework. Indeed, hydrodynamics predicts that the HCS is unstable with respect to long-wavelength fluctuations of the velocity field. The repercussions on the behavior of a mixture have not been explored to date. We verified that $K_1(t)$ and $K_2(t)$ exhibit—separately—the t^{-2} and t^{-1} scaling behaviors that are commonly observed in one-component systems.

Figure 2 shows that $\gamma = K_1/K_2$ changes rather sharply from the initial plateau value of the HCS to a higher plateau value. The number of collisions at which the crossover occurs is proportional to $(1 - r^2)^{-1}$ and diverges when the system approaches perfect elasticity. As we mentioned above, the position of the lower plateau is well accounted for by the BE theory. From Fig. 2 one can also see that the asymptotic, higher plateau corresponds

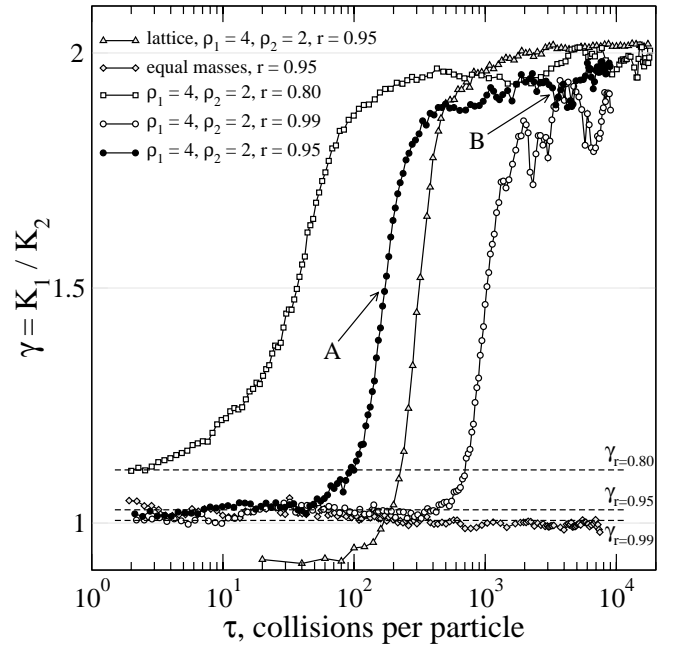


FIG. 2. Ratio of the kinetic energies of the two species for different values of the coefficient of restitution. The crossover from $K_1/K_2 \sim 1$ to $K_1/K_2 \sim m_1/m_2$ is clearly visible. For comparison, we also show the corresponding result for the lattice model. The status of the system at points A and B is shown in Fig. 1.

to $K_1/K_2 = m_1/m_2$. This correspondence was confirmed for several values of the density ratio of the two species. Whereas in the HCS the inelasticity determines only a small departure from equipartition, in the intermediate and late regimes such a breakdown becomes more severe: the specific asymptotic value of γ means that particles with different masses eventually share the same velocity distributions; i.e., “equipartition” of velocities eventually sets in. Although not previously reported, the phenomenon has a simple explanation: due to the inelasticity of collisions, the velocities of the particles tend to become more and more parallel. Since momentum conservation does not allow the velocities to select a unique direction, the velocity field develops many vortices (see Fig. 1), i.e., a situation of local alignment. The occurrence of a collision depends only on the relative velocities of particles, and not on their masses, coefficients of restitution, or other properties. Therefore, the velocity of a given particle tends to be locked to the velocity of neighbors, regardless of their species. The fact that the ratio K_1/K_2 eventually attains the value m_1/m_2 is a striking manifestation of the long range velocity correlations that develop in a granular fluid. We checked the above argument against a different case, wherein densities are kept unchanged and the masses of the two species are made equal by choosing different radii for them. The result is shown in Fig. 2 (gray diamonds). In this case the value of γ stays close to $m_1/m_2 = 1$. Also, the dependence on

other parameters (such as coefficient of restitution, geometrical factors, and tangential friction modeled as in Ref. [12]) was found to be rather weak. Of course, real granular materials are subject to more complex dissipative forces. Our tests, however, show that γ asymptotically depends mainly on m_1/m_2 , although the detailed crossover dynamics reflects the specific parameters.

It is interesting to observe that the previously presented scenario is reproduced by a very simple extension to mixtures of the inelastic lattice model of Ref. [10]. The mixture consists of N_1 and N_2 “particles” with the same physical properties as above, sitting randomly on the $M = N_1 + N_2$ nodes of a 2D triangular lattice. Every particle is characterized by a 2D vector velocity \mathbf{v}_i , but its position stays fixed. A dynamics is induced by randomly choosing two neighboring particles and updating their velocities according to the rule of Eq. (1). The free streaming component of the dynamics is neglected, but velocity correlations are properly taken into account. After an exponential decay, the energy decreases as $K \sim \tau^{-d/2}$, as usual. Correlations become more and more important as time elapses, showing the presence of a growing length scale $L(\tau) \sim \tau^{1/2}$ associated with the average diameter of the vortices [10]. As shown in Fig. 2 (gray triangles) the lattice mixture model can reproduce the asymptotic value of γ . To demonstrate that velocity correlations are responsible for the specific value of γ , we shuffled the velocity of each particle right after collision, by exchanging its velocity with that of a randomly chosen particle. This suppresses completely the $\tau^{-d/2}$ energy decay, the vortex instability, and the crossover in γ .

In the third stage of cooling, density fluctuations lead to cluster formation, as in monodisperse systems. In addition to that (see Fig. 4), we observe a novel and appreciable segregation of species, which we quantify by studying the following ratios S_1 and S_2 of integrated (partial) pair distribution functions: $S_\alpha = \int_0^D g_{\alpha\alpha}(r) r dr / \int_0^D g_{\alpha\beta}(r) r dr$, where $g_{\alpha\beta}(r)$ ($\alpha, \beta = 1, 2$) are the partial pair correlation functions and D is a cutoff distance, here chosen equal to $5R$. Figure 3 shows the time evolution of S_1 and S_2 for different choices of the mass ratio. For values of τ corresponding to the transition in γ (refer to Fig. 2), local segregation appears: heavy particles tend to group together ($S_1 > 1$), and the effect increases with the mass ratio. A simple heuristic argument can explain such a finding. The average change of kinetic energy $\langle \Delta E_\alpha \rangle_\beta$ of a particle of species α colliding with a particle of species β can be expressed as a function of the local kinetic temperatures [13] T_1 and T_2 as [14]

$$\langle \Delta E_\alpha \rangle_\beta = \frac{m_\alpha m_\beta}{(m_\alpha + m_\beta)} \frac{(1+r)}{2\sqrt{2}} \times \left[(1+r) \frac{T_\beta m_\alpha + T_\alpha m_\beta}{m_\alpha (m_\mu + m_\beta)} - 2 \frac{T_\alpha}{m_\alpha} \right]. \quad (2)$$

One sees that particles with a smaller mass gain energy

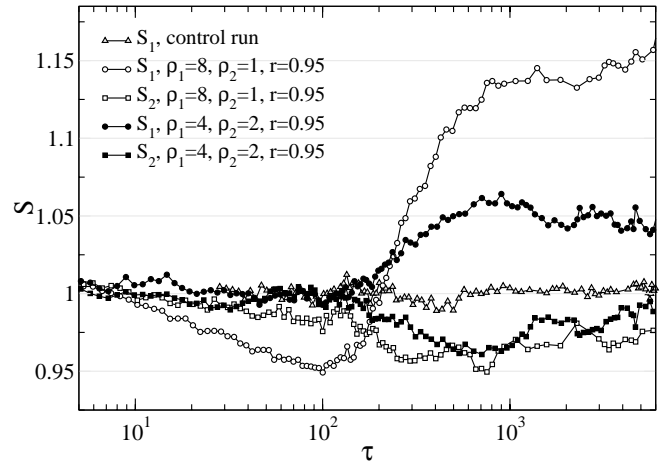


FIG. 3. Local segregation: the temporal evolution of the ratios S_1 and S_2 of integrated correlation functions (see text) is shown for $m_1/m_2 = 2$ and $m_1/m_2 = 8$. To assess noise levels, a control run with $m_1 = m_2$ is also shown.

($\langle \Delta E_2 \rangle_1 > 0$) at the expenses of the heavy particles, provided that $T_1/T_2 > [(1-r)m_1/m_2 + 2]/(1+r) > 1$. Indeed, our numerics confirm that this condition is satisfied for our system. For a perfectly elastic system there is no energy transfer, since $T_1 = T_2$. In the dissipative case, instead, since the ratio of the kinetic temperatures $T_1/T_2 > 1$, light particles—on average—gain kinetic energy when colliding with heavy particles. This results in an effective repulsion of the light particles by the heavy

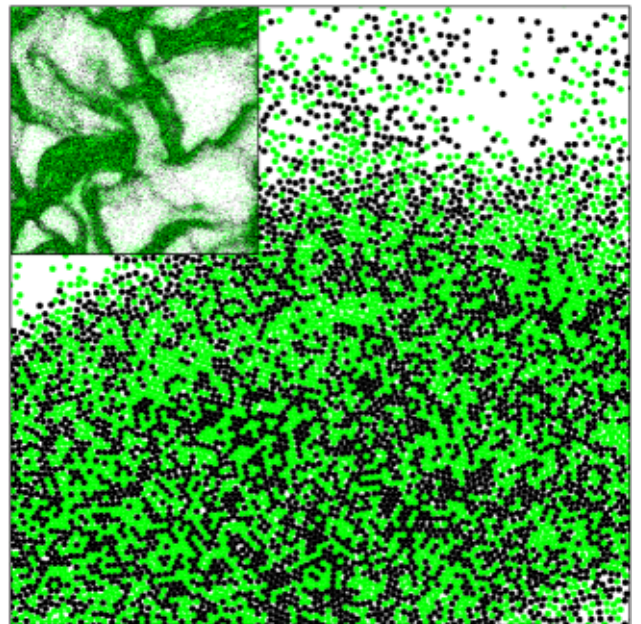


FIG. 4 (color online). Composition pattern within a cluster after $\tau = 1300$ collisions per particle, for $r = 0.95$ and $m_1/m_2 = 8$. Black disks correspond to heavier particles. The radius of the particles is $R = 0.1$ cm. Inset: global state of the system.

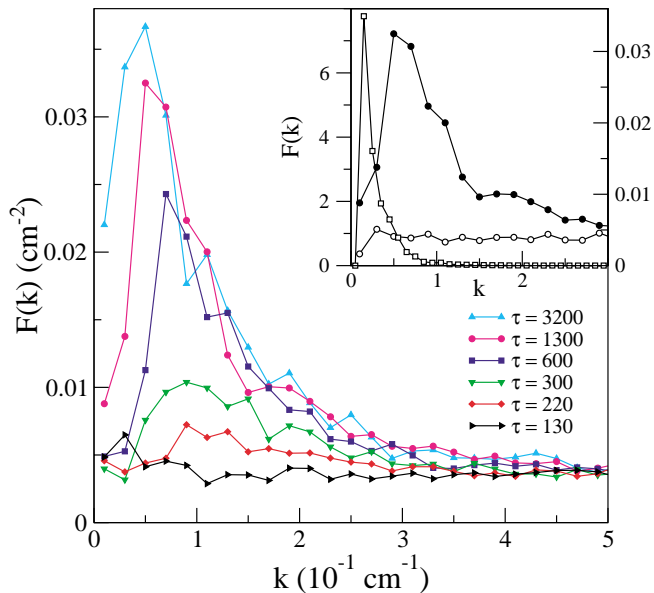


FIG. 5 (color online). Circularly averaged composition structure factor, $F(k, t)$, at different times. With time, the peak grows higher and moves towards smaller wave vectors. The inset shows how the peak for $\tau = 1300$ (solid circles, right vertical axis) is suppressed on reshuffling the particle species (empty circles, right axis). The structure factor of the total density field (empty squares, left axis) has a peak at a much lower wave vector. For these curves, $r = 0.95$ and $m_1/m_2 = 8$, as in Fig. 4.

ones. The above scenario is also consistent with the asymmetry between species observed in the temporal evolution of the indicators $S_{\alpha,\beta}$ of local segregation.

Such a microscopic mechanism driving segregation has also global effects. Let us consider the long-wavelength properties of the composition field $\phi(\mathbf{r}, t) \equiv n_1(\mathbf{r}, t) - n_2(\mathbf{r}, t)$, the difference of the local number densities of the two species, whose dynamics is slow due to its conservative nature. The analysis of the structure factor $F(\mathbf{k}, t) = \hat{\phi}(\mathbf{k}, t)\hat{\phi}^*(\mathbf{k}, t)$ [where $\hat{\phi}(\mathbf{k}, t)$ is the Fourier transform of $\phi(\mathbf{r}, t)$] reveals a remarkable scenario: at the onset of clustering the uniform composition state becomes unstable and evolves into an interconnected pattern of domains with different composition, as shown in Fig. 4. Long-wavelength fluctuations of $\phi(\mathbf{r}, t)$ are amplified and—contrary to the usual diffusion processes—particles of different species tend to segregate. The temporal evolution of the above (circularly averaged) structure factor is reported in Fig. 5. In the homogeneous stage of cooling, the structure factor is featureless (right triangles). When clustering appears, a broad peak develops (diamonds) and with time it grows higher, while shifting towards low wave vectors. Reshuffling the

particle species—while keeping their positions unchanged—suppresses the peak altogether, as shown in the inset of Fig. 5. This proves that the above spectral properties are truly a manifestation of progressive, long-wavelength ordering of the two species. Moreover, the peak in $F(k, t)$ is unrelated to the short wave vector peak that—because of clustering—is expected in the structure factor of the total density field (see the Fig. 5 inset): the composition field and the density field have very different characteristic lengths.

In conclusion, we found that the strong velocity correlations induced by inelasticity result in a ratio of kinetic energies $K_1/K_2 \approx m_1/m_2$ that is not accounted for by the BE theory, which underestimates the effect of dynamical correlations. This can be regarded as a manifestation of the noise reduction effect [15] of granular systems, where a suitable collective arrangement of the velocities minimizes dissipation. In addition to that, in the clustered stage, segregation builds up according to a phenomenology which bears similarities to the spinodal decomposition occurring in metallic alloys, where a growing characteristic length appears in the composition field.

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