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# Pattern Formation in the Inhomogeneous Cooling State of Granular Fluids

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We present results from comprehensive event-driven (ED) simulations of nonlinear pattern formation in freely-evolving granular gases. In particular, we focus on the the morphologies of density and velocity fields in the inhomogeneous cooling state (ICS). We emphasize the strong analogy between the ICS morphologies and pattern formation in phase ordering systems with a globally conserved order parameter.

There has been much recent interest in the properties of powders or granular materials [1, 2]. These materials are of great scientific and technological relevance and display properties intermediate to those of solids and fluids. Perhaps the most relevant feature of powders is that the grains dissipate energy on collision. Therefore, granular materials exhibit interesting dynamical properties only when the collisional energy loss is compensated by a continuous input of energy [1, 2].

It is also relevant to investigate the dynamical evolution of a freely-evolving homogeneous system of inelastic granular particles. In the initial stages, the system continuously loses energy in a homogeneous cooling state (HCS), where the density field is approximately uniform [3]. However, the HCS is unstable to density fluctuations, and the system evolves into an inhomogeneous cooling state (ICS), where particle-rich clusters are formed and grow [4]. There is a good understanding of the HCS and the instabilities which result in the ICS [3, 4, 5, 6]. However, there is only a limited understanding of the nonlinear evolution of the ICS [7, 8]. In this letter, we study nonlinear domain growth processes for the granular density and velocity fields in the asymptotic time-regime. We present results from comprehensive event-driven (ED) simulations for a wide range of inelasticity and density parameters. In particular, we invoke analogies from studies of phase ordering dynamics [9, 10] to obtain a *quantitative* characterization of the evolving morphologies in the ICS. The similarities between freely-evolving granular gases and phase ordering systems have been briefly discussed by Van Noije, Ernst and co-authors [6], and Baldassari *et al.* [8]. Of course, we stress that the mechanisms driving pattern evolution are very different in both cases.

We consider a system of identical inelastic hard spheres (with mass $m = 1$ and diameter $\sigma = 1$) in a $d = 2$ box of size $(N_b\sigma)^2$, with periodic boundary conditions. There is no external input of energy in our simulations. We use an event-driven algorithm [11], which only keeps track of particle collisions, to evolve the system. After a collision between the $i^{th}$ and $j^{th}$ particles, having velocities $\vec{v}_i$ and $\vec{v}_j$ respectively, the new velocities are $\vec{v}_i' = \vec{v}_i - \frac{1+e}{2}[\hat{n}\cdot(\vec{v}_i - \vec{v}_j)]\hat{n}$, $\vec{v}_j' = \vec{v}_j + \frac{1+e}{2}[\hat{n}\cdot(\vec{v}_i - \vec{v}_j)]\hat{n}$. Here, $\hat{n}$ is the unit vector parallel to the relative position of the particles. For elastic collisions, we have the coefficient of restitution $e = 1$. For granular materials, $e < 1$ in general.

The initial condition for each run consisted of $N$ particles with a homogeneous spatial distribution and a Maxwellian velocity distribution. For circular particles, the average pack-

ing fraction is $\phi = \pi N/(4N_b^2)$. We always fix $N_b = 256$ and vary $N$, as specified below. We will label our results using the number fraction, $n = N/N_b^2$. Numerical data are obtained for the following parameter sets: (i) $N = 30000$ (or $n \simeq 0.46, \phi \simeq 0.36$), and $e$ ranging from 0.80 to 0.975 in steps of 0.025; (ii) $e = 0.90$, and $N$ ranging from 10000 to 40000 in steps of 5000, i.e., $n \simeq 0.15$ to 0.61. We characterize the dynamical evolution of the granular gas using various statistical quantities, which are calculated as an average over 5 independent runs, i.e., correlation functions, structure factors, and domain growth laws for the density and velocity fields.

For early times, inelastic collisions result in cooling as $\frac{dT(t)}{dt} = -\frac{\epsilon}{d}\omega(T)T$, where $T(t)$ is the temperature at time $t$; $\epsilon = 1 - e^2$; and $\omega(T)$ is the collision frequency at temperature $T$ [3]. The form of $\omega(T)$ is approximately determined from the Enskog theory for elastic hard spheres as $\omega(T) \simeq \omega(T_0)(T/T_0)^{1/2}$, where $T_0$ is the granular temperature at $t = 0$. This yields Haff's cooling law for the HCS [3] as $T(t) = T_0 \left[1 + \frac{\epsilon\omega(T_0)}{2d}t\right]^{-2} = T_0 e^{-\frac{\epsilon}{d}\tau}$, where $\tau(t)$ is the average number of collisions per particle upto time $t$. Our subsequent results are presented in terms of $\tau$, as this constitutes a reasonable measure of time in the present context. The values of $\tau$ are obtained directly from the ED simulations. We should stress that $\tau(t)$ vs. $t$ fluctuates considerably for individual runs in the ICS regime.

In Fig. 1, we show evolution snapshots for the $d = 2$ granular gas with $n \simeq 0.46$. The LHS and RHS frames refer to the coarse-grained velocity field $\vec{v}(\vec{r}, \tau)$ and density field $\psi(\vec{r}, \tau)$, respectively. The coarse-grained fields at a lattice point are obtained by averaging over boxes of size $(5\sigma)^2$ centered at that point. To clarify the nature of pattern formation, we have "hardened" the velocity field in Fig. 1, i.e., the length of all vectors has been set to unity. Points where the velocity field is zero, due to the absence of particles in the coarse-graining box, are unmarked in Fig. 1. The density field on the RHS of Fig. 1 is depicted in a binary representation. We introduce the order parameter $\psi(\vec{r}, \tau)$ with values $+1$ $(-1)$ at points where the number density is larger (less) than the average number density.

The upper frames in Fig. 1 correspond to $e = 0.85$ and $\tau = 150$. The velocity field is characterized by the emergence and diffusive coarsening of vortices. There is a progressive parallelization of the local velocity field due to inelastic dissipation of the normal velocity components. However, as the total momentum is fixed at zero and the system is doubly-periodic, defects will be present in the velocity field for all times. Typically, pattern evolution in the density field is slower than that for the velocity field [6]. Nevertheless, well-defined

clusters corresponding to the ICS are already seen at $\tau = 50$ (not shown here). These clusters grow with time in a manner reminiscent of phase ordering systems [9]. The vortex centers in the velocity field are also shown (as black circles) in the frame on the RHS. The vortex density diminishes with time, and vortices are primarily confined to regions of low density, as there is a rapid parallelization of velocities in the high-density (solid-like) region due to multiple collision processes. There is no strong correlation between the location of defects in the velocity field (i.e., vortices) and defects in the density field (i.e., interfaces or domain boundaries). The middle frames in Fig. 1 correspond to $e = 0.90$. The broad features are the same as those for $e = 0.85$, though the time-scales are slower. All time-scales for pattern formation diverge as $e \to 1$, i.e., the clustering instability is delayed for more elastic systems. The perfectly elastic case ($e = 1$) is singular, and does not exhibit clustering.

A coarse-grained description of the granular fluid is provided by nonlinear hydrodynamic equations for the density, velocity and temperature fields, in conjunction with an energy loss term [4]. Wakou *et al.* [12] have shown that fluctuations in these quantities obey TDGL-like equations of phase ordering dynamics with a nonconserved order parameter [10]. Typically, these equations are obtained as the overdamped limit of a Hamiltonian formulation. In this letter, we clarify the TDGL-description of granular dynamics.

The evolution of the density field is analogous to phase ordering dynamics in two-component (AB) mixtures, which is described by the equation [10]:

$$\frac{\partial \psi(\vec{r},t)}{\partial t} = (-\nabla^2)^m \left[\psi(\vec{r},t) - \psi(\vec{r},t)^3 + \nabla^2 \psi(\vec{r},t)\right], \tag{1}$$

where $\psi(\vec{r},t)$ differentiates between $A$-rich ($\psi = +1$) and $B$-rich ($\psi = -1$) regions. Eq. (1) with $m = 0$ is the TDGL equation, and describes nonconserved systems. In this case, the coarsening system is characterized by a diffusive growth law, $L(t) \sim t^{1/2}$ [9, 10], where $L(t)$ is the characteristic domain size at time $t$. On the other hand, Eq. (1) with $m = 1$ is the Cahn-Hilliard (CH) equation, and describes conserved systems. In this case, the domain growth process obeys the Lifshitz-Slyozov (LS) law, $L(t) \sim t^{1/3}$ [9, 10]. Finally, there have also been studies of Eq. (1) with $m \to 0^+$, which is referred to as the globally-conserved (GC) TDGL equation [13]. This model is known to be in the same dynamical universality class as the nonconserved TDGL equation [13], with the difference that the initial composition is preserved in the GC-TDGL equation.

Similarly, the evolution of the velocity field in the ICS is comparable to ordering dynamics

in the XY model, which is the vector version of Eq. (1):

$$\frac{\partial\vec{\psi}(\vec{r},t)}{\partial t} = (-\nabla^2)^m \left[\vec{\psi}(\vec{r},t) - |\vec{\psi}(\vec{r},t)|^2\vec{\psi}(\vec{r},t) + \nabla^2\vec{\psi}(\vec{r},t)\right], \tag{2}$$

where $\vec{\psi} \equiv (\psi_1, \psi_2)$. The evolution in Eq. (2) parallelizes $\vec{\psi}$ locally via the annihilation of vortices and anti-vortices, driven by a surface-tension reduction mechanism. Eq. (2) with $m = 0$ corresponds to the case with nonconserved order parameter. The corresponding domain growth law [14] is $L_v(t) \sim t^{1/2}$. On the other hand, Eq. (2) with $m = 1$ corresponds to the conserved XY model, where the dynamics locally conserves $\vec{\psi}$.

The evolution of the granular fluid conserves both the density and velocity fields. Intuitively, one may expect that the analogous phase ordering models would be the conserved ($m = 1$) versions of Eqs. (1)-(2). However, the evolution morphologies in the upper and middle frames of Fig. 1 are comparable to those for the case with nonconserved order parameter [9]. This is a consequence of the non-diffusive dynamics of granular particles, which move in straight lines until they collide with other particles. In this collision, the density and momentum are conserved quantities, of course. However, depending on the density of the fluid, the distance traveled by particles prior to collision may be considerable. Therefore, the variables are conserved on the macroscopic length-scale of the mean-free path, and not on the microscopic length-scale of the lattice spacing. Now, the ICS consists of regions of high density and low density. Granular particles stream relatively unhindered through the low-density regions and deposit on distant clusters. Typically, the conservation length scale is comparable to the length scale of the coarsening clusters, which diverges in time. Therefore, the density and velocity fields are globally conserved (GC), rather than locally conserved. To elucidate this analogy, the lower LHS frame in Fig. 1 shows the velocity field from the GC-XY model with $\langle\vec{\psi}\rangle = 0$. The lower RHS frame in Fig. 1 shows the density field for the GC-TDGL model with $\langle\psi\rangle = -0.08$, corresponding to an average density of 0.46.

Before we quantify the morphologies in Fig. 1, we would like to study the HCS $\rightarrow$ ICS crossover time. Brito and Ernst [15] use mode-coupling techniques to obtain the asymptotic energy decay (in the ICS) as

$$T(\tau) \simeq \frac{T_0}{2n}\left(\frac{d-1}{\xi_\perp^d} + \frac{1}{\xi_{||}^d}\right)\left(\frac{4\pi\epsilon}{d}\tau\right)^{-d/2}, \tag{3}$$

where $\xi_\perp \simeq \sqrt{\frac{2d}{\epsilon}} l_0$ and $\xi_{||} \simeq \frac{2d}{\epsilon} l_0$, with $l_0$ being the time-independent mean-free path. A comparison of Haff's law and Eq. (3) yields the crossover time $\tau_c$ as the solution of

$$\tau_c^{d/2} e^{-\frac{\epsilon}{d}\tau_c} \simeq \frac{(d-1)}{2} \left(\frac{\Omega_d}{4\pi}\right)^d \chi(n)^d n^{d-1}, \tag{4}$$

where $\sigma = 1$, and $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the $d$-dimensional solid angle. We consider the case $\epsilon \to 0$, so that $\xi_{||} \gg \xi_\perp$. For $d = 2$, Eq. (4) simplifies as $\tau_c e^{-\frac{\epsilon}{2}\tau_c} \sim n\chi(n)^2$, where we ignore prefactors. We use the Verlet-Levesque approximation for the $d = 2$ hard-sphere correlation function at contact, viz., $\chi(n) = (1 - 7\phi/16)(1-\phi)^{-2}$. In Fig. 2(a), we plot $e^{\frac{\epsilon}{2}\tau_c}$ vs. $\tau_c$ for $n \simeq 0.46$ and a range of $e$-values. In Fig. 2(b), we plot $\tau_c e^{-\frac{\epsilon}{2}\tau_c}$ vs. $n\chi(n)^2$ for $e = 0.90$ and a range of $n$-values. These approximately linear plots confirm the validity of the scaling behavior of $\tau_c(e, n)$, as expected from Eq. (4).

Next, we examine the time-dependent structure factors of the density and velocity fields in the ICS. The evolving morphologies are characterized by unique length scales, and we expect the structure factors to exhibit dynamical scaling, i.e., $S(k, \tau) = \ell(\tau)^d f(k\ell)$, where $\ell$ is the relevant length scale and $f(x)$ is a scaling function [10]. In Fig. 3(a), we plot the scaled structure factors of the density field for $(n, e) = (0.46, 0.85)$, i.e., $\ln[S_{\psi\psi}(k,\tau)\langle k\rangle^2]$ vs. $\ln(k/\langle k\rangle)$ from three different times ($\tau \gg \tau_c$). The quantity $\langle k\rangle$ is the first moment of the structure factor, and is related to the length scale as $\langle k\rangle^{-1} \sim L(\tau)$. The reasonable data collapse confirms the validity of dynamical scaling. The dashed line in Fig. 3(a) denotes the Fourier transform of the analytic result due to Ohta *et al.* (OJK) [16] for the correlation function of the nonconserved TDGL equation: $g(x) = \frac{2}{\pi}\sin^{-1}(\gamma)$, where $\gamma = e^{-x^2}, x = r/L$. The OJK function provides an excellent description of our numerical data. The dot-dashed line in Fig. 3(a) is obtained from a numerical simulation of the CH equation with $\langle\psi\rangle = -0.08$. The CH result is at variance with our numerical results except for the tail region. In particular, the local conservation law dictates that $S_{\rm CH}(k,t) \sim k^4$ as $k \to 0$ [10]. However, the ICS structure factor appears to decay almost monotonically from $k = 0^+$, as is usual for structure factors in ordering problems characterized by a nonconserved order parameter. (Of course, global density conservation dictates that $S_{\psi\psi}(0,\tau) = 0$.) Fig. 3(b) is analogous to 3(a), but corresponds to the case with $e = 0.90$.

We have confirmed numerically that the scaled structure factor for the density field in the ICS has only a weak dependence on the off-criticality $\langle\psi\rangle$, which measures the average density. Furthermore, it is numerically comparable to the OJK function for a broad range

of $\langle\psi\rangle$-values. The nature of defects in the ordering field dictates some general properties of the structure factor. For example, scattering off interfaces in the density field gives rise to a power-law (or Porod) decay in the structure factor tail, $S_{\psi\psi}(k,\tau) \sim k^{-(d+1)}$ for large $k$ [17], which is seen clearly in Figs. 3(a)-(b).

In Figs. 4(a)-(b), we plot scaled structure factors, $\ln[S_{vv}(k,\tau)\langle k\rangle^2]$ vs. $\ln(k/\langle k\rangle)$, for the velocity field in the ICS. The dashed line denotes the Fourier transform of the Bray-Puri-Toyoki (BPT) function for ordering in the nonconserved XY model [14]:

$$h(x) = \frac{n\gamma}{2\pi}\left[B\left(\frac{n+1}{2},\frac{1}{2}\right)\right]^2 F\left(\frac{1}{2},\frac{1}{2};\frac{n+2}{2};\gamma^2\right), \tag{5}$$

where $\gamma = e^{-x^2}, x = r/L_v$; $B(x,y)$ is the beta function; and $F(a,b;c;z)$ is the hypergeometric function. The BPT result corresponds to defects with $O(n)$ symmetry, and the case with $n = 2$ is relevant here. Again, we see that our numerical data is described well by the BPT function, and is completely different from the result for the conserved XY model (obtained numerically, and denoted as a dot-dashed line in Figs. 4(a)-(b)).

We have seen that vortex defects characterize the morphology of the ICS velocity field. These vortices give rise to a power-law decay for the structure factor tail, $S_{vv}(k,\tau) \sim k^{-(d+2)}$ for large $k$. The general BPT result in Eq. (5) exhibits a power-law tail, $S(k,t) \sim k^{-(d+n)}$, and is relevant for the ICS in granular systems with $d > 2$.

For the time-regimes considered here, a description in terms of two uncoupled order parameters is reasonable. A more complete description of the asymptotic ordering dynamics should account for *holes* in the velocity field due to absence of particles in some regions of space. This is provided by a model with spin-vacancy phase separation in conjunction with XY-like ordering of the spin variable. In the current context, the relevant model has coupled nonconserved (or globally conserved) dynamics for the two ordering fields. At a later stage, we will discuss in detail the applicability of this model to the ICS.

Finally, we would like to briefly discuss domain growth laws in the ICS. We should stress that late-stage dynamics is affected by inelastic collapse, where a group of particles undergo an infinite number of collisions in a finite time [18]. The results discussed here correspond to the regime prior to inelastic collapse. Subsequent to the HCS $\rightarrow$ ICS crossover, our numerical results (not shown here) are consistent with diffusive growth, $L(\tau), L_v(\tau) \sim \tau^{1/2}$ [6]. Furthermore, our numerical data is consistent with an asymptotic power-law behavior, $\tau(t) \sim t^{2/3}$, for a wide range of parameter values. Therefore, in real time, the length scales

behave as $L(t), L_v(t) \sim t^{1/3}$ [7]. The domain growth law for the ICS density field is the same as the LS growth law for phase separation of binary mixtures.

In conclusion, we have undertaken comprehensive ED simulations of nonlinear pattern formation in the density and velocity fields of an inelastic granular gas. We find that there is a close analogy between ICS morphologies and phase ordering systems with globally conserved order parameters. The nature of defects in the ordering fields dictates general properties of the relevant structure factors and correlation functions. Furthermore, our numerical results for the structure factors of the ICS density and velocity fields are described well by analytic results for nonconserved phase ordering systems. Clearly, the general formalism of phase ordering dynamics is of great utility in diverse problems of pattern formation as many features of evolution morphologies are determined by general principles, e.g., defect structures, conservation laws, etc.

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## Figure Captions

**Figure 1:** Evolution pictures for the coarse-grained density and velocity fields in the ICS. The upper RHS frame shows the density field at $\tau = 150$ for $(n, e) = (0.46, 0.85)$. Regions with density greater than the average are marked in grey. The black circles denote the vortex centers of the velocity field. The upper LHS frame shows the direction vectors of the corresponding velocity field. For clarity, we only show a $32^2$ corner (as depicted in the RHS frame) of the $256^2$ lattice. The middle frames are the density and velocity fields at $\tau = 150$ for $(n, e) = (0.46, 0.90)$. The lower RHS frame shows an evolution picture (at $t = 25$) for the GC-TDGL equation with $\langle\psi\rangle = -0.08$, corresponding to average density 0.46. The lower LHS frame shows an evolution picture (at $t = 25$) for the GC-XY model with $\langle\vec{\psi}\rangle = 0$.

**Figure 2:** Dependence of $\tau_c$ on system parameters. The crossover time is obtained from energy-decay plots (not shown here) as the point of deviation from Haff's law. The error bars are defined by the symbol sizes. (a) Plot of $e^{\frac{\epsilon}{2}\tau_c}$ vs. $\tau_c$ for $n \simeq 0.46$; and $e$ ranging from 0.80 to 0.95. The solid line denotes the best linear fit to the data. (b) Plot of $\tau_c e^{-\frac{\epsilon}{2}\tau_c}$ vs. $n\chi(n)^2$ for $e = 0.90$; and $n$ ranging from 0.08 to 0.53.

**Figure 3:** (a) Scaled structure factors for the coarse-grained density field for $(n, e) = (0.46, 0.85)$. Data is plotted for $\tau(\gg \tau_c) = 100, 150, 250$. (b) Analogous to (a), but for $(n, e) = (0.46, 0.90)$.

**Figure 4:** Analogous to Fig. 3, but for the coarse-grained velocity field.

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