Cooling of a lattice granular fluid as an ordering process

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We present a microscopic model of granular medium to study the role of dynamical correlations and the onset of spatial order induced by the inelasticity of the interactions on the velocity field. In spite of its simplicity and intrinsic limitations, it features several aspects of the rich phenomenology observed in granular materials and allows to make contact with other topics of statistical mechanics such as diffusion processes, domain growth, aging phenomena. Interestingly, while local observables, being controlled by the largest wavelength fluctuations, seem to suggest a purely diffusive behavior, the formation of spatially extended structures and topological defects, such as vortices and shocks, reveals a more complex scenario. Finally, only for quasielastic systems, we observe a neat scale separation, which represents a fundamental hypothesis to develop a granular hydrodynamics.

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The effort devoted during the last decades to investigate off equilibrium systems has achieved a series of successes by virtue of a combination of experiments, numerical simulations, exact theoretical results and clever phenomenological arguments, but our comprehension of the area is far from complete. Among these systems granular materials (GM), i.e., assemblies of macroscopic particles that dissipate their energy through inelastic collisions and frictional forces, have acquired a special rank due to their complex phenomenology often intriguing and only partly understood [1]. For instance, granular gases [2] may behave very differently from ordinary fluids constituted by elastic particles.

Years ago, Ulam showed that an ensemble of elastic particles, starting from an arbitrary configuration, converged to a Maxwell equilibrium distribution, postulating a simple redistribution law of the kinetic energies of randomly selected pairs to simulate the effect of binary collisions in an elastic gas [3]. Ben-Naim and Kaprivski (BK), recently, introduced a variation over this theme, by letting the particles endowed with a scalar velocity to dissipate inelastically a fraction of the relative kinetic energy at each collision [4]. The master equations associated to these models correspond to a class of solvable Boltzmann equations, known as Maxwell models [5], which recently have attracted a vivid interest in the case of inelastic interactions [6], due to the discovery of an asymptotic exact scaling solution [7]. Nevertheless, since Maxwell models fulfill the molecular chaos hypothesis, rule out the formation of dynamical correlations.

In fact, during the cooling of a granular gas [2], such correlations are negligible in a first well studied dynamical regime, called "homogeneous cooling." On the other hand molecular dynamics (MD) simulations have shown the appearance of a shear instability (i.e., vortices in the velocity field), which breaks the homogeneous cooling process. The later appearance of density clusters increases the complexity of the dynamics [8]. In an interesting series of papers, van Noije and collaborators have put forward a mesoscopic theory of these phenomena, making a connection with phase ordering kinetics [9]. They predict that the shear instability always precedes the cluster instability, as indicated by MD simulations. Unfortunately, such simulations are quite demanding, preventing a definitive check of the results and the limits of their hydrodynamic theory, which still lacks of a full microscopic justification.

In the present work we shall introduce and study a microscopic model that preserves the simplicity of Ulam's approach, and displays a complexity similar to that observed in granular systems. The focus of our study will be on the statistics of the velocity field and on its spatial and temporal correlations, stressing the analogies and the differences with related models aimed to describe off equilibrium systems. We shall also consider the issue of a hydrodynamic description of granular flows, exploring the existence of a well separated mesoscopic scale.

Our model, which reduces to an inelastic Maxwell model in a mean field treatment of correlations, is suited to study the density-homogeneous cooling regime. This may be a limitation, with respect to existing models of inelastic gases [10], but allows a direct comparison with MD simulations, where the density cluster instability can be avoided by an appropriate choice of external fields or boundary conditions [9]. On the other hand, our model represents, perhaps, the minimal correction to the molecular chaos assumption that can lead to progress in the theory of simple kinetic models.

We introduce our dynamical model by associating a d-dimensional velocity field $\mathbf{v}_i$ with each node of a d-dimensional lattice; at each time step a nearest neighbor pair (i,j) is randomly selected and the two velocities are updated according to the rule,

$$\mathbf{v}_j' = \mathbf{v}_j + \Theta(-(\mathbf{v}_i - \mathbf{v}_j)\hat{\sigma})\frac{1+\alpha}{2}[(\mathbf{v}_i - \mathbf{v}_j)\hat{\sigma}]\hat{\sigma},$$

$$\mathbf{v}_i' = \mathbf{v}_i - \Theta(-(\mathbf{v}_i - \mathbf{v}_j)\hat{\sigma})\frac{1+\alpha}{2}[(\mathbf{v}_i - \mathbf{v}_j)\hat{\sigma}]\hat{\sigma} \qquad (1)$$

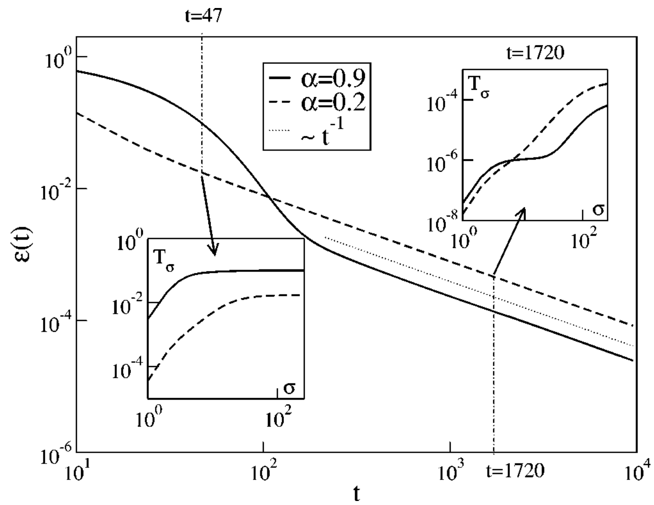

FIG. 1. Energy decay for $\alpha=0.9$ and $\alpha=0.2$ (1024^2 sites). In the insets we reported the scale dependent temperature T_σ as a function of the coarse graining size σ for $t=47$ and $t=1720$.

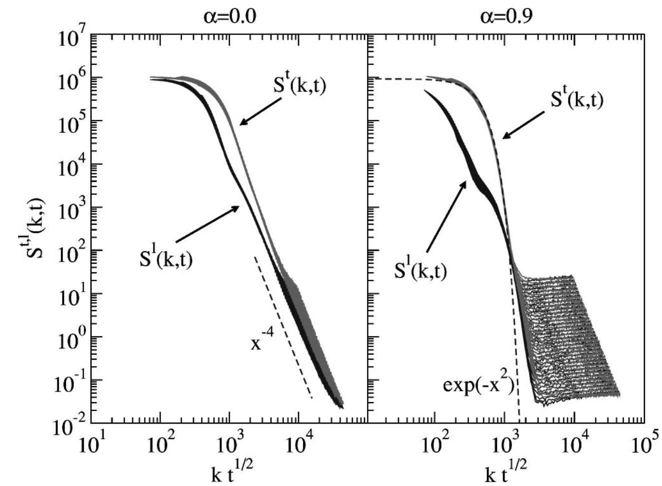

FIG. 2. Data collapse of the transverse (S^t) and longitudinal (S^l) structure functions for $\alpha=0$ and $\alpha=0.9$ (system size 1024^2 sites, times ranging from $t=500$ to $t=10^4$). For comparison we have drawn the laws x^{-4} and $\exp(-x^2)$.

where $\hat{\sigma}$ represents the unit vector pointing from site i to j, Θ is the Heaviside function that enforces the kinematic constraint and α the normal restitution parameter. We shall measure time in the nondimensional number of collisions per particle. In each elementary collision [see Eq. (1)] the total linear and angular momentum are conserved, whereas a fraction $(1-\alpha^2)/4$ of the relative kinetic energy is dissipated. The inelasticity of the collisions has the effect of reducing the quantity $|(\mathbf{v}_i-\mathbf{v}_j)\hat{\sigma}|$, i.e., induce a partial alignment of the velocities. Hereafter we report the study performed in two dimensions on a triangular lattice.

The freely cooling process exhibits striking similarities with the quench from an initially stable disordered phase to a low temperature phase in a magnetic system: whereas in a standard quench process [11] one considers the process by which a system, brought out of equilibrium by a sudden change of an external constraint, such as temperature or pressure, finds its new equilibrium state, in a GM one wants to study the relaxation of a fluidized state, after the external driving force (whose role is to reinject the energy dissipated by the collisions) is switched off at time $t=0$. The rotational symmetry of the order parameter $\mathbf{v}_i$ and the momentum conserving interaction determine the presence of many configurations having comparable dissipation rates. Due to their competition the system does not relax immediately towards a motionless state, but displays a phenomenology similar to that observed in a coarsening process.

One sees from Fig. 1 that during the initial stage, the average energy per particle $\epsilon(t)=\Sigma v_i(t)^2/N$ is dissipated at an exponential rate $\tau^{-1}=(1-\alpha^2)/4$. This can be deduced from Eq. (1) imposing that each "spin" fluctuates independently of the others. For times larger than $t_c\sim\tau$, the dynamics enters a different regime, where the cooperative effects become dominant and the average energy per particle decays as $\epsilon(t)\sim t^{-1}$ [12].

The first exponential decay is well known and corresponds to Haff's homogeneous cooling law, while the second regime agrees with recent simulations of inelastic hard spheres [13]. As shown below, the crossover from one regime to the other is due to the formation of a macroscopic velocity field. This is analogous to the formation of magnetic domains in standard quench processes. After the formation stage these regions start to compete to homogenize, causing a conversion of kinetic energy into heat by viscous heating, i.e., act against the collisional cooling and lead to a slower decay [9].

Within the early regime the velocity distribution deviates sensibly from a Maxwell distribution (corresponding to the same average kinetic energy), but displays fatter tails. Whereas large tails are reproduced by several theoretical approaches that neglect spatial correlations (as in the BK model or Boltzmann equation), the behavior of the velocity distribution when correlations emerge is unknown. In our model, when the energy begins to decay as t^{-1}, the velocity distribution turns Gaussian [14].

The most relevant information about the spatial ordering process is contained in the equal-time structure functions, i.e., the Fourier transforms of the velocity correlation function,

$$S^{t,l}(k,t)=\sum_{\hat{k}} v^{t,l}(\mathbf{k},t)v^{t,l}(-\mathbf{k},t)$$

where v^t and v^l indicate, respectively, the transverse and longitudinal components of the field with respect to the wave vector $\mathbf{k}$ and the sum $\Sigma_{\hat{k}}$ is over a circular shell of radius k. Using our model, we can compute such structure factors with a high precision. A fairly good data collapse is observed in terms of the variable $(kt^{1/2})$, apart from the large k region, which identifies two growing lengths $L^{t,l}(t)$ (see Fig. 2). Considering the sum rule $\epsilon(t)=\Sigma_k[S^t(k,t)+S^l(k,t)]$ we observed that in the early "exponential" regime the contribution from the two terms is approximately equal, whereas for times larger than t_c and α not too small most of the kinetic energy remains stored in the transverse field, while the longitudinal component decays faster, with an apparent exponent t^{-2}.

The findings concerning the energy decay, the distribution of the velocity field, and the growth of $L^{t,l}(t)$, lead to the conclusion, that, if the observation time is longer than the time between two collisions and if the spatial scale is larger than the lattice spacing, the system behaves as if its evolution were governed by a diffusive dynamics [9]. To be more precise, let us consider a vector field $\vec{\phi}(x,t)$ that evolves according to the law $\partial_t \vec{\phi} = \nu \nabla^2 \vec{\phi}$ starting from a random uncorrelated initial condition. The explicit solution shows that $\vec{\phi}(x,t)$ is asymptotically Gaussian distributed, with a variance $\langle \vec{\phi}(x,t)\vec{\phi}(x,t)\rangle \propto t^{-d/2}$. The structure factors $S^{t,l}(k,t)$ assume a scaling form $S^{t,l}(k,t) = s(kL(t))$ where $L(t) = \sqrt{t}$.

Furthermore, we compared the two-time autocorrelation $C(t_1,t_2) = \Sigma_i \mathbf{v}_i(t_1)\mathbf{v}_i(t_2)/N$ with $C_\phi(t_1,t_2) = \langle \phi(x,t_1)\phi(x,t_2)\rangle$, whose expression reads: $C_\phi(t_1,t_2) = 2\, C_\phi(t_1,t_1) \times (1 + t_1/t_2)^{-1}$. During a short time transient, the autocorrelation function of our model differs from C_ϕ, since it depends on $t_1 - t_2$, i.e., it is time translational invariant (TTI). Later, $C(t_1,t_2)$ reaches the "aging" regime and depends only on the ratio $x = t_1/t_2$. Something similar occurs in a coarsening process, where the autocorrelation of the local magnetization $a(t_w, t_w+\tau)$ reaches, for large τ (but $\tau \ll t_w$), a constant value $m_{eq}^2(T)$, that is the square of the equilibrium magnetization. Obviously, for $T \to 0$, $m_{eq}^2 \to 1$ and the TTI transient regime disappears. The short time transient in our model is analogous to such a TTI regime, with the peculiar difference that the cooling process imposes a decreasing temperature $T(t_w) \to 0$, that progressively erodes the TTI regime. The same dependence on the TTI manifests itself in the angular autocorrelation: $A(t,t_w) = \Sigma_i \cos[\theta_i(t+t_w) - \theta_i(t_w)]/N$. Again, for large waiting times t_w this function assumes the diffusive t/t_w scaling form, but for a small fixed t_w, displays a minimum and a small peak before decreasing at larger t (see Fig. 3). The interesting nonmonotonic behavior of $A(t,t_w)$ suggests that the initial direction of the velocity induces a change in the velocities of the surrounding particles, which in turn generates, through a sequence of correlated collisions, a kind of retarded field oriented as the initial velocity. As t_w increases the maximum is less and less pronounced.

In spite of these first results, that seem to give support to the idea that the model dynamics is purely diffusive the model is more complex. The main evidence stems from the following facts: (i) the structure functions do not have the typical Gaussian tails of a diffusive system, due to the nonlinearity represented by the kinematic factor in Eq. (1) and the shapes of $S^{t,l}(k,t)$ display three different regions: a long-wavelength region that is diffusive in character; an intermediate region where the structure functions decay as $k^{-\beta}$ with $\beta \sim 4$; a plateau region where $S^{t,l}$ decay in time with a power law t^{-2} but remains nearly constant with respect to k (for $\alpha > 0$); (ii) the Fourier modes interact and an initial shear state, obtained assuming the initial configuration to be a plane wave, decays into shorter wavelength modes by a mechanism of period doubling; that is to say, contrary to the diffusion, plane waves are not eigenmodes.

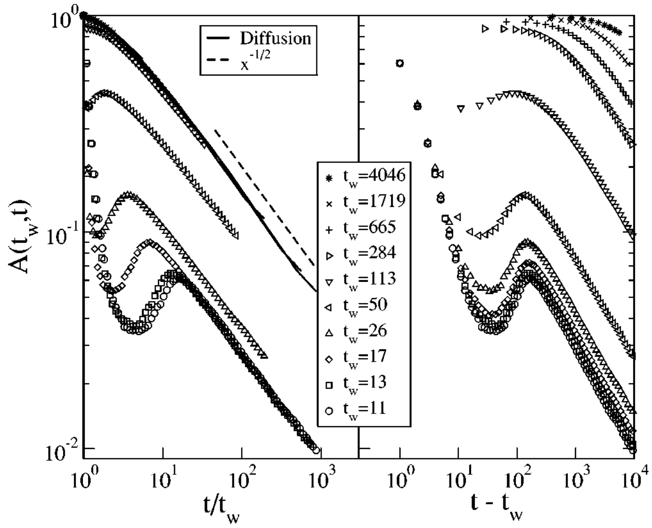

FIG. 3. Angular autocorrelation function $A(t,t_w)$ for different values of the waiting time t_w and $\alpha = 0.9$ (1024^2 sites). The graph on the left shows the convergence to the t/t_w diffusive scaling regime, for large t_w. For small t_w, a local minimum is visible (for such a quasielastic dynamics). In the graph on the right the same data are plotted vs $t - t_w$: note that the small t_w curves tend to collapse. For higher t_w the position of the local minimum does not move sensibly, but its value grows and goes to 1 for large t_w.

The existence of the quasielastic plateaux is the fingerprint of localized fluctuations which, for small inelasticity, propagate and are damped less than exponentially. A small α determines a rapid locking of the velocities of neighboring elements to a common value, while in the case of $\alpha \to 1$, short range small amplitude disorder persists within the domains, breaking simple scaling of $S^{t,l}$ for large k and having the effect of a self-induced noise. The presence of an internal noise, never directly measured in MD IHS simulations, is invoked in fluctuating hydrodynamic theories [9]. It would be interesting to characterize such internal noise by means of an average local granular temperature T_σ, i.e., a measure of the variance of $\mathbf{v}_i$ with respect to the local average of $\mathbf{v}$ within a region of linear size σ. Obviously, since when $\sigma \to \infty$ the local average tends to the global (zero) momentum, then $T_\sigma \to \epsilon$, as shown in the insets of Fig. 1. For $\sigma < L(t)$, instead, $T_\sigma < \epsilon$. For quasielastic systems T_σ exhibits a plateau for $1 \ll \sigma \ll L(t)$ that identify the strength of the internal temperature. Such a local temperature ceases to be well defined for smaller α due to the absence of scale separation between microscopic and macroscopic fluctuations in the strongly inelastic regime [15].

The existence of a $L^{-2}(t)k^{-4}$ region in the structure functions is consistent with Porod's law [11] and is the signature of the presence of vortices, a salient feature of the cooling process. Vortices form spontaneously and represent the boundaries between regions that selected different orientations of the velocities during the quench and are an unavoidable consequence of the conservation laws that forbid the formation of a single domain. With the random initial condi-

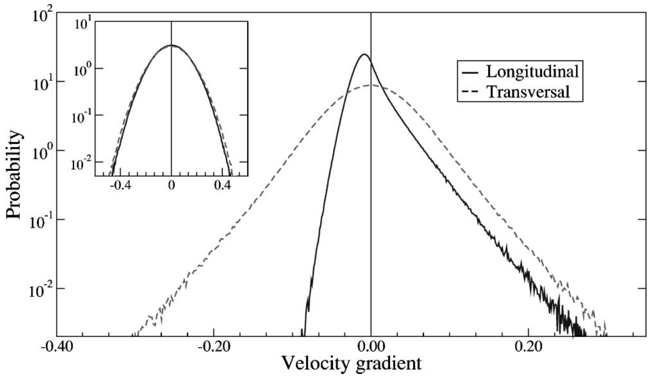

FIG. 4. Probability densities of the longitudinal and transverse velocity increments. The main figure shows the PDF of the velocity gradients ($R=1$). The inset shows the Gaussian shape measured for $R=40$ [larger than $L(t)$ for this simulation: $\alpha=0.2$, $t=620$, system size 2048^2].

tions adopted, vortices are born at the smallest scales and subsequently grow in size by pair annihilation, conserving the total charge.

Vortices are not the only topological defects of the velocity field. In fact, shock fronts in the velocity field of driven rapid granular flows have been recently observed in experiments [16]. For the cooling case, evidence in one-dimensional simulations [17] has raised several interesting questions with respect to the connection with Burgers equation in higher dimensions [13,18].

In our two-dimensional simulations, we observe shocks as shown by the distributions of the velocity longitudinal increments:

$$\Delta_l(\mathbf{R}) = \frac{1}{N}\Sigma_i(\mathbf{v}_{i+R}-\mathbf{v}_i)\cdot\mathbf{R}/R.$$

.

The pair distribution functions (PDF's) are shown in Fig. 4 for $R=1$ (longitudinal velocity gradient) in the main frame, and for $R=40>L(t)$ in the inset. For small $R\ll L(t)$ the longitudinal increment PDF is skewed with an important positive tail, whereas for $R\gg L(t)$ it turns Gaussian. The distribution of transverse increments $(\mathbf{v}_{i+R}-\mathbf{v}_i)\times\hat{\mathbf{R}}$, instead, is always symmetric, but non-Gaussian distributed for small R. A similar situation exists in fully developed turbulence [19].

To conclude, our model provides a link between the microscopic rules of granular dynamics and its hydrodynamical description. It allows to follow the cooling of a granular material and the buildup of velocity correlations, by means of efficient numerical measures of structure factors, two-time correlations and topological defects. The data analysis reveals the presence of vortices, shocks, and internal noise and suggests the existence of a scale separation only in the case of quasielastic systems, which is instead suppressed for large inelasticities.

Even independently of the problem of granular flows, the model represents a simple but unusual phase ordering system. In fact, despite the apparently purely diffusive aspects shown by one-point quantities, it displays anomalous statistics of spatial properties for the order parameter field as witnessed by the velocity gradient PDF and by the structure functions.

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