Aging and multiscaling in out of equilibrium dynamical processes of granular media

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In the framework of recently introduced frustrated lattice gas models, we study the out of equilibrium dynamical processes during the compaction process in granular media. We find irreversible-reversible cycles in agreement with recent experimental observations. Moreover in analogy with the phenomenology of the glass transition we find aging effects during the compaction process. In particular we find that the two time density correlation function $C(t,t')$ asymptotically scales as a function of the single variable $\ln(t')/\ln(t)$. This result is interpreted in terms of multiscaling properties of the system.

The experimental study of dynamic processes in granular media has recently revealed the presence of interesting behaviours. Under tapping dry granular media reach very slowly a more compact state which is well fitted by a logarithmic relaxation. More recently Novak et al. have also shown that such materials exhibit non trivial irreversible-reversible cycles. These phenomena stem from slow relaxation processes due to large “cooperative rearrangements” of many particles. In such a perspective granular materials share features of thermal systems such as glasses or spin glasses which are also characterized by extremely long relaxation times and the presence of irreversible-reversible cycles.

In this paper in the framework of recently introduced microscopic models, we reproduce the irreversible-reversible cycles of Novak et al. and investigate the effect of the “cooling” rate on the compaction process. We find a behaviour which is strongly reminiscent of the phenomenology of the glass transition. Finally we study the non equilibrium time dependent density density autocorrelation function and found aging effects typical of glassy systems. These results suggest that similar effects could be also found in real experiments.

In dynamical processes of granular media a crucial role is played by geometric frustration (originated by steric hindrance between interlocked neighboring grains) which induce the necessity of large scale cooperative rearrangements for relaxation. Based on these concepts two kinds of frustrated lattice gas model were introduced. Both models showed logarithmic compaction, segregation and other phenomena typical of granular media under shaking.

These models consist of a system of particles which occupy the sites of a square lattice tilted by $45^\circ$ (see Fig.1). Particles are characterized by an internal degree of freedom, $S_i = \pm 1$, corresponding for instance to two typical orientations of grains on the lattice. Two nearest neighbor sites can be both occupied only if the particles have the right reciprocal orientation, so that they do not overlap, otherwise, due to excluded volume, they have to move away. In absence of vibrations the particles are subject only to gravity and they move downwards always fulfilling the non overlap constraint. The effect of vibration is introduced by allowing the particles to diffuse with a probability $p_{up}$ upwards and a probability $p_{down} = 1 - p_{up}$ downwards. An important parameter governing the dynamics is the adimensional parameter $\Gamma \equiv -1/\ln(x_0)$, with $x_0 = p_{up}/p_{down}$, which is related (see below) to the effective temperature of the system and consequently plays the same role as the amplitude of the vibration intensity in the experiment of Novak et al.

Such models can be described in terms of the following lattice gas Hamiltonian (see Fig.1) in the limit $J \to \infty$:

$$H = J \sum_{\langle ij \rangle} f_{ij}(S_i, S_j)n_in_j$$

Here $n_i = 0,1$ are occupancy variables, $S_i = \pm 1$ are spin variables, associated to the two orientations of the particles, $J$ represents the infinite repulsion felt by the particles when they have the wrong orientations and $f_{ij}(S_i, S_j) = 0$ or $1$ depending whether the configuration $S_i, S_j$ is right (allowed) or wrong (not allowed).

The choice of $f_{ij}(S_i, S_j)$ depends on the particular model. The Tetris model is made of elongated particles (see Fig.1), which may point in two directions coinciding with the two lattice bond orientations. In this case $f_{ij}(S_i, S_j)$ is given by $f_{ij}(S_i, S_j) = 1/2(S_iS_j - \epsilon_{ij}(S_i + S_j) + 1)$, where $\epsilon_{ij} = +1$ for bonds along one direction of the lattice and $\epsilon_{ij} = -1$ for bonds on the other. This hamiltonian model has an ordered “antiferromagnetic”
ground state, and its dynamics has the crucial constraint that particles can flip their “spin” only if 3 of their own neighbors are empty.

A real granular system may contain more disorder due to a wider shape distribution or to the absence of a lattice. Therefore in a more realistic model the number of internal states is \( q > 2 \) (\( S_i = 1, 2, ..., q \)) and the function \( f_{ij}(S_i, S_j) \) is zero only for allowed nearest neighbor configurations.

However to simplify the model the number of states was still kept \( q = 2 \) and the randomness was taken into account by introducing random quenched variables corresponding to the freezing of some degree of freedom in the high density regime. Thus an Ising frustrated lattice gas model (IFLG) was proposed \([7]\) in which the Hamiltonian (1) is without gravity. In presence of gravity there is an extra term \( g \sum_i n_i y_i \) where \( g \) is the gravity and \( y_i \) is the ordinate of the particle \( i \). The temperature \( T \) is related to the ratio \( x_0 = p_{up}/p_{down} \) via \( e^{-2g/T} = x_0 \), (notice \( \Delta = T/2g \)).

Interesting enough the two extreme models, the Tetris and the IFLG, show similar behaviour. This suggests that the results found are rather robust and will not depend much on the details of the model. In particular under tapping they reproduce the logarithmic behaviour in agreement with the experimental results of Knight et al. \([3]\). Experimentally a “tap” is the shaking of the container of the grains by vibrations of given duration and amplitude. In our Monte Carlo simulations each single tap is realized by letting the particle diffuse under the gravity by keeping \( \Gamma = \text{const.} \) during the time interval of a tap, \( \tau_0 \), and then switching off the vibration by setting \( \Gamma = 0 \) until the system reaches a static configuration. Time \( t \) is measured in such a way that one unit corresponds to one single average update of all particles and all spins of the lattice.

In a previous paper \([6]\) we have performed on the IFLG a particular cycle sequence of taps to show the presence in granular media of hysteresis effect. Recently also real experiments were performed on density relaxation in granular media under cyclic tapping \([6]\), which show indeed the presence of such hysteresis effect. In order to compare better with the experimental data we have simulated the same cycle of Novak et al. on the IFLG model. We have considered a system of size \( 30 \times 60 \) (our data are robust to size changes), with periodic boundary conditions along the x-axis and rigid walls at bottom and top. Our data are averaged over 8 different lattice realizations each averaged over 30 different noise realizations.

A starting particle configuration is prepared by randomly inserting particles into the box from its top and then letting them fall down, with the dynamics described above, until the box is filled. We performed cycles of taps in which the vibration amplitude \( \Gamma \) is varied at fixed amplitude increment \( \gamma = \Delta \Gamma / \tau_0 \) holding constant their duration \( \tau_0 \). More precisely we performed a sequence of \( N \) taps, of amplitude \( \Gamma_1, ..., \Gamma_N \), from an initial amplitude \( \Gamma_1 = 0 \) to a maximal amplitude \( \Gamma_{\text{max}} = 15 \), then back to \( \Gamma = 0 \) and then up again to \( \Gamma_N = \Gamma_{\text{max}} \). After each tap we measure the static bulk density of the system \( \rho(\Gamma_n) \) (\( n \) is the n-th tap number).

Our results are qualitatively very similar to those reported in real experiments on dry granular packs \([6]\). We find that when the system is successively shaken at increasing vibration amplitudes, the bulk density of the system typically grows and then decreases as shown in Fig. \([3]\). However, when the amplitude of shaking decreases back, the density follows the same path only up to some value of \( \Gamma \) and then deviates from it, in fact it does not bend down and keeps growing. As in the experimental data the second part of the shaking cycle is approximately reversible (see Fig. \([3]\)). For such a reason these processes are called “irreversible-reversible” cycles \([3]\). Interestingly the reversible cycle is a monotonic function of the shaking amplitude (see Fig. \([3]\)).
To study the dependence on the “cooling” rate $\gamma$, we repeated the tapping sequence for different values of the tap amplitude increment $\Delta \Gamma$ with a fixed tap duration $\tau_0$ (see Fig. 3). We find that the reversible branches have a common part for high values of $\Gamma$ while for small $\Gamma$ they splits in different curves depending on the cooling rate $\gamma$. The slower the cooling rate the higher is the final density observed at the end of the descending part of the cycle. One can schematically define the point, $\Gamma_0(\gamma)$, where the system freezes and goes out of equilibrium as the location of the “shoulder” in these “reversible” branches (see Fig. 3). Thus, $\Gamma_0(\gamma)$, which depends on $\gamma$, corresponds to a “glass transition”. Notice that $\Gamma_0(\gamma)$ is usually different from the point, $\Gamma^*(\gamma)$, where the “irreversible” and the “reversible” branches meet (see Fig. 3). However, as $\gamma$ gets smaller $\Gamma_0$ and $\Gamma^*$ become closer and they may coincide in the limit $\gamma \to 0$.

![Figure 3](image)

**FIG. 3.** As in Fig. 2, we report the density, $\rho(\Gamma)$, as a function of the vibration amplitude, $\Gamma$ for three different values of the “cooling” velocity $\gamma$. For sake of clarity, we plot here only the descending reversible parts of the cycle. As in experiments on glasses a too fast cooling drives the system out of equilibrium. The position of the shoulder, $\Gamma_0(\gamma)$, in these curves schematically individuates a “glass transition”.

As in glasses the system gets out of equilibrium due to the fact that the characteristic times of relaxation are much larger than the time $\tau_0$ involved in the experiment, but, for the same reason, the location of the path depends on the rate $\gamma$.

The limit of $\gamma$ going to zero defines an ideal glass transition amplitude $\Gamma_0$. Using the analogy with the glass transition we expect a slow logarithm dependence of $\Gamma_0(\gamma)$ on $\gamma$ as in the glass transition. Full details will be presented elsewhere [10]. Experimental results in this direction will be also very interesting.

By further exploiting the analogy with the glass transition, we expect aging phenomena. For instance if one keep shaking the system at a low fixed amplitude $\Gamma$ on the reversible branch, the system will slowly (logarithmically) approach an asymptotic value of the density, eventually on the equilibrium curve. In order to further quantitatively characterize the out of equilibrium dynamics and aging phenomena in granular matter and make quantitative predictions, in analogy with glassy system we introduce a two time density-density correlation function ($t \geq t'$):

$$C(t, t') = \frac{\langle \rho(t)\rho(t') \rangle - \langle \rho(t) \rangle \langle \rho(t') \rangle}{\langle \rho(t')^2 \rangle - \langle \rho(t') \rangle^2}$$

where $\rho(t)$ is the bulk density of the system at time $t$. In out of equilibrium $C(t, t')$ is a function of both times $t$ and $t'$ (at equilibrium just of $t-t'$). The aging properties of the system are characterized by the specific scaling properties of $C(t, t')$.

In order to study the system in a well defined configuration of its parameters, we evaluate $C(t, t')$ during a “single tap”: we prepare the system at $t = 0$ by randomly pouring grains in the box from above as described before, then we start to shake it continuously and indefinitely with a given (small) amplitude $\Gamma$. We expect very similar results by considering, instead of a long tap, a series of short taps which is experimentally more convenient (as in ref. [4]). The data about $C(t, t')$ we present here are averaged, at least, over 8 different lattice and 512 different noise realizations.

At low $\Gamma$, a good fit for the two time correlation function, $C(t, t')$, on the whole five decades in time explored, is given by the following:

$$C(t, t') = (1 - c_\infty)\frac{\ln[(t' + t_s)/\tau]}{\ln[(t + t_s)/\tau]} + c_\infty$$

where $\tau$, $t_s$ and $c_\infty$ are fit parameters. Very interesting is the fact that the above behavior is found in both of our models (Tetris and IFLG). The data for the two models, for several values of $\Gamma$, rescaled on a single universal master function, are plotted in Fig. 4. In particular, in the explored range of $\Gamma \in [0.11, 0.43]$ (i.e., $x_0 \in [10^{-4}, 10^{-1}]$), we found $\tau \sim e^z/\Gamma$ (with $z \sim 2$ in both the IFLG and the Tetris), the mark of activated dynamics ($t_s(\Gamma)$ behaves approximately as $\tau$ as a function of $\Gamma$). The asymptotic value $c_\infty$ is difficult to determine with some precision: in the above $\Gamma$ range we evaluated approximately $c_\infty = 0.2 \div 0.3$ for the IFLG model and $c_\infty = 0.0 \div 0.2$ for the Tetris model.

Eq. (3) essentially states that for times long enough the correlation $C(t, t')$ is a function (linear) of the ratio $\ln(t'/\tau)/\ln(t)$. Such a scaling behaviour is known in others disordered systems like Random Ferromagnets or Random Fields models [11] and has been proposed by Fisher and Huse droplets theory of finite dimensional spin glasses [12]. However, it seems to be different from other scaling functions proposed to fit experimental data.
in spin glasses. All this shows the necessity of experimental confirmation of our results in the framework of granular media.

In any case, eq. (3) is in good agreement with a general multiscaling approach presented in Refs. [13,14]. Whenever the characteristic relaxation times of the system becomes exceedingly large with respect to those typical of the measurements, it is reasonable to assume scaling properties for the system. The most general scaling transformation which satisfies group properties gives rise to a multiscaling form of the correlation function given by [14]:

\[ C(t, t') = C(\alpha) t^{f(\alpha)} \quad (4) \]

with a twofold possibility for \( \alpha \): \( \alpha = t'/t^z \) or \( \alpha = \ln(t')/\ln(t) + O(1/\ln(t)) \); here \( C(\alpha) \) and \( f(\alpha) \) are two generic functions. The assumption of multiscaling might thus naturally allow to explain the presence of large classes of universality found in scaling behaviour of apparently different systems. The above case of eq. (3), observed in both Tetris and IFLG, corresponds to \( \alpha = \ln(t')/\ln(t) \) and \( f(\alpha) \sim 0 \).

In conclusion, in the framework of simple frustrated lattice gas models, we have studied the off equilibrium dynamics of slightly shaken granular materials. These models have previously shown to share many phenomena characteristic of granular media as logarithmic compaction or segregation. Here, we have studied irreversible-reversible cycles and found good agreement with the experimental data on granular packs.

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