

## A model for the compaction of granular media

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We introduce a lattice model, in which frustration plays a crucial role, to describe relaxation properties of granular media. We show Monte Carlo results for compaction in the presence of vibrations and gravity, which compare well with experimental data.

Despite their importance for industrial applications relaxation phenomena in non-thermal disordered systems as granular media, have just recently begun to be studied systematically. A common and simple experiment in this context, is the compaction of sand. When a box filled with loose packed sand is shaken at low amplitude, density visibly increases. If in addition the density goes beyond a definite threshold the mechanical properties of sand abruptly change and the granular structure cannot be sheared any longer without a volume increase. This phenomenon, very important in practical applications [1], was observed by Reynolds [2] and is referred to as the "Reynolds" or "dilancy" transition.

For a given macroscopic parameter as density a granular packing can be in a huge number of different microscopical states. In order to describe this situation concepts from statistical mechanics have been introduced [3–5]. Relations to spin glasses (SG) have been suggested several years ago (see references in [3]). In fact a characteristic of SG is their non trivial phase space which gives rise to its complex static and dynamic behavior. The phase space structure of SG is due to the presence of quenched disorder and frustration. Strictly speaking quenched disorder is not present in granular media but there are effects of "geometric frustration", known also from hard sphere systems. This kind of frustration is generated by the steric constraints imposed by the hard core repulsion of neighboring grains and the subsequent interlocking which leads to non local cooperative macroscopic rearrangements. Recently the analogies between an intrinsically frustrated system like frustrated percolation [6] and phase transitions in a granular packing have been outlined [7].

In this paper we present computer simulations of a simple frustrated Ising lattice gas model, subject to gravity following a diffusion like Monte Carlo dynamics. The particles in this system are characterized by internal degrees of freedom which describe their orientation or other local sterical properties of the grains. This model without gravity shows complex behavior similar to the one observed in glass forming liquids and spin glasses [8]. We

will show how the density of our lattice gas is strongly dependent on the duration and the amplitude of simply implemented vibrations. Our data reproduce the logarithmic relaxation behavior found in real experiments in a sequence of taps and offer the possibility to make new predictions also for single tap processes. Our data also reproduce the distribution of forces at the bottom of the system as found in real experiments. A relation appears between the SG transition, signaled by the vanishing of macroscopic self-diffusion, and the Reynolds transition in granular systems.

We consider a system of particles which move on a square lattice whose bonds are characterized by quenched random numbers  $\epsilon_{ij} = \pm 1$ . On site  $i$  we set  $s_i = 1$  if a particle is present and 0 otherwise. The particles have an internal degree of freedom  $S_i = \pm 1$  and are subjected to the constraint that whenever two ( $i$  and  $j$ ) are neighboring, their "spin" must satisfy the relation

$$\epsilon_{ij} S_i S_j = 1 \quad (1)$$

i.e. they have to fit the local "geometrical" structure. When the density of particles is high enough they can feel the frustration that has been imposed by the choice of the  $\epsilon_{ij}$ . As a consequence, in resemblance to frustrated percolation [6], particles can never close a frustrated loop in the lattice leaving empty sites (see below).

The physical origin of the bond variables  $\epsilon_{ij}$ , is the geometrical frustration originated in granular systems by the actual shapes and arrangements of particles and the internal variables  $S_i$  mimic local shapes and positions.

We have studied this system when subject to "gravity" and "external vibrations". The dynamics of our model consists in a random diffusion of particles on a square lattice tilted by  $45^\circ$  (see Fig.1) in such a way as to preserve the above constraint. The particles attempt a move upward with probability  $P_2$  and downward with  $P_1$  (with  $P_1 + P_2 = 1$ ). The move is made only if the internal degree of freedom satisfy eq. (1). Similarly a spin flips with probability one if there is no violation of eq. (1), and does not flip otherwise. In absence of vibrations, the effect of gravity imposes  $P_2 = 0$ . When vibrations are switched on  $P_2$  becomes finite. The crucial parameter which controls the dynamics and the final density is the ratio  $\alpha(t) = P_2(t)/P_1(t)$  which describes the amplitude of the vibration.

It is possible to associate to this model a standard Hamiltonian formalism and establish a magnetic analogy,

based on the following definition:

$$-H = \sum_{\langle ij \rangle} J(\epsilon_{ij} S_i S_j - 1) n_i n_j + \mu \sum_i n_i \quad (2)$$

where  $S_i = \pm 1$  are spin variables,  $n_i = 0, 1$  occupancy variables and  $\epsilon_{ij} = \pm 1$  quenched interactions associated to the bonds of the lattice. It has been shown in mean field approximation [9] and numerically for finite dimensional systems [8], that Hamiltonian (2) exhibits a spin glass transition at high density (or low temperature).

This Hamiltonian reduces in the  $\mu \rightarrow \infty$  limit (all sites occupied) to the usual  $\pm J$  Ising spin glass [10]. In the limit  $J \rightarrow \infty$ , it describes a lattice gas in which frustrated loops entirely filled with sites are forbidden because along closed paths energetic reasons impose the quantity  $\sum_{i,j \in \text{loop}} (\epsilon_{ij} S_i S_j - 1)$  to be zero. In this limit a version of *site frustrated percolation* is recovered [6,8]. When the particle number is fixed the configuration space of the system obtained in this last limit is the same as that of the frustrated lattice gas introduced at the beginning of this paragraph.

We have studied the model introduced above in a 2D box with periodic boundary conditions along the x-axis and rigid walls at its bottom and top.

After fixing the random quenched  $\epsilon_{ij}$  on the bonds, a random initial particle configuration is prepared by randomly inserting particles of given spin into the box from its top and then letting them fall down, with the described dynamic ( $P_x = 0$ ), until the box is filled. To obtain an initial standard configuration with low and uniform density, in this preparation process we do not allow particle spins to flip. The state so defined has a density of about 0.520 and corresponds to a sort of random loose packing.

We know experimentally that sand which is randomly poured into a box reaches higher density after shaking.

In some experiments, the shaking process occurs in a sequence of "taps". A "tap" is the shake, with a vibration exciter, of a box filled with grains. The "shape" of a tap is defined by its duration and its amplitude. After a sequence of taps the density decays to its static limit logarithmically (see [11]). We have studied the phenomena of density relaxation during a sequence of taps. In our MC simulation, each tap is a process in which vibrations are step like:  $\pi(t) = \pi_0$  if  $t \in [0, \tau]$  while for  $t > \tau$  the system evolves subject only to gravity ( $P_x = 1$  and  $P_y = 0$ , i.e.  $\pi(t) = 0$ ) until it reaches a final "static" configuration [12]. After each tap we have measured the bulk density of the system  $\rho(\tau, \pi_0; i_n)$  defined as the mean density in the lower 25% of the box ( $i_n$  is the  $n$ -th tap number). Our results for density relaxation, in a box of size  $30 \times 60$  averaged over 32 different  $\{\epsilon_{ij}\}$  configurations, are shown in Fig. 2. The behavior of  $\rho(\tau, \pi_0; i_n)$  is well fitted by the following logarithmic function in agreement with the experimental data (see [11,13]):

$$\rho(\tau, \pi_0; i) = \rho_s - \Delta \rho_{\infty} / [1 + B \ln(i/\tau_0 + 1)] \quad (3)$$

We have also simulated a single tapping process. In this case we have found that the relaxation, instead of being logarithmic as in the sequence of taps is well described by a "stretched exponential". In the simulation we start at  $t = 0$  from a random loose packing configuration described before, then we introduce "vibrations" in the interval  $t \in [0, \tau]$  linearly decreasing the ratio  $\pi(t)$ ,  $\pi(t) = \pi_0(1 - t/\tau)$  (with  $\pi_0 = 1$ ). For  $t > \tau$  we put  $\pi(t) = 0$  and let the system evolve until it reaches a final "static" configuration. The final "static" bulk density  $\rho(\tau)$  monotonically increases with the vibration time  $\tau$  asymptotically reaching a maximal density value  $\rho^* \sim 0.78$  when  $\tau \rightarrow \infty$  [14].

This effect of compaction is clearly shown by the final density profile as a function of depth  $h$ ,  $\rho(h, \tau)$ , depicted in Fig. 3. In this case the box has a size  $100 \times 200$  and the final states have been averaged over 32 to 512 different  $\{\epsilon_{ij}\}$  configurations (according the value of  $\tau$ ). As suggested in ref. [15] the density profile of granular media can be fitted using a generalised Fermi-Dirac distribution. As shown in Fig. 3 the data from our model are well fitted by such a function for different values of  $\tau$ :

$$\rho(h, \tau) = \rho_s(\tau) [1 - 1 / [1 + \exp((h - h_0(\tau))/s(\tau))]] \quad (4)$$

During the dynamical process described above, we have recorded the time dependence of the mean bulk density  $\rho(t, \tau)$ . We find that the static limit is reached with a stretched "relaxation form" [14]:

$$\rho(t, \tau) = \rho_s(\tau) - A \exp(-((t - t_0)/T)^\beta) \quad (5)$$

Typical values of the parameters of eq. (5) in our range of  $\tau$  are  $A \in [0.15, 0.25]$ ,  $t_0 \in [-10^4, 10^3]$ ,  $T \in [10^2, 10^4]$ ,  $\beta \in [2, 4]$ . Note that the stretched exponential behavior only sets in after a time  $t_0$ , which can be very long if  $\tau$  is long. The relaxation processes found here are rather different from the logarithmic relaxation found in the sequence of taps and could be investigated experimentally.

To characterize a particle packing and its capability of internal rearrangement, we studied their self-diffusivity at fixed global particle density by setting  $\pi = 1$ . Specifically we have studied the time dependence of the particle mean square displacement  $R^2(t) = \langle \frac{1}{N} \sum_i (r_i(t) - r_i(0))^2 \rangle$ .

A very interesting phenomena is observed for densities close to the maximal value  $\rho^*$ :  $R^2(t)$  shows deviations from the linear time dependence typical of standard Brownian diffusive motion and presents an inflection point [8]. This signals the existence of two characteristic time regimes for particle motion (as already argued in [16]). From the long time behavior of  $R^2(t) \sim Dt$  we extract the diffusion coefficient  $D(\rho)$ , which goes to zero at about  $\rho^*$ , signalling a localisation transition in which particles are confined in local cages and the macroscopic diffusion-like processes are suppressed. This phenomena may also be described in a different way:  $\rho^*$  is the density above which it becomes impossible to obtain a macroscopic rearrangement of the particle positions without increasing the system volume, i.e. the density at which

macroscopic shear in the system is impossible without dilatancy. This then seems to correspond to the quoted Reynolds transition in real granular media.

The density  $\rho^*$  coincides with the density at which the spin glass (SG) transition of Hamiltonian (2) (for  $J \rightarrow \infty$ ) is located. This implies that at  $\rho^*$  the SG correlation length  $\xi_{SG}$  diverges, signalling the presence of collective behavior in the system. In SG this length can be detected by measuring the non linear susceptibility. In granular material the spin variables represent internal degree of freedom and cannot be easily detected.

The coincidence of the SG transition and the suppression of self-diffusivity suggest the equivalence of the Reynolds transition in granular media, the SG transition in magnetic systems and the "ideal" glass transition in glass forming liquids [7,8]. Like in glass forming liquids the Reynolds transition does not show divergences in thermodynamic functions.

The model here introduced is suited to study also other aspects of granular media phenomenology. If a force is applied at the top of a granular system in a box, the distribution of forces  $\sigma$  at the bottom follows an exponential law  $P(\sigma) = a \cdot \exp(-c \cdot \sigma)$ . As suggested in [17-19], it is possible to introduce simplified models to describe the physics of forces in granular systems. In particular in [18] has been proposed a model in which forces may be dealt with as substantially scalar quantities and a crucial element is randomness in grain packing. In our lattice model we apply this kind of concepts to study forces distributions in static configurations of the system. We suppose that each present site ( $n_i = 1$ ) carries his own weight (equal to unity) and transmits the force acting on it,  $w_i$ , to his first two neighboring sites in the lower row. If its right (left) neighbor has a distance  $l_r$  ( $l_l$ ) from it, the force contribution it receives from site  $i$  is equal to  $w_i \cdot l_l / (l_r + l_l)$  (resp.  $w_i \cdot l_r / (l_r + l_l)$ ). We have calculated the force distribution  $P(\sigma)$  at the bottom of our system as shown in Fig. 1. In agreement with the experimental data and the result of the model introduced in [18], our data are well fitted by:

$$P(\sigma) = a \cdot \sigma^b \exp(-c \cdot \sigma) \quad (6)$$

As noted in Ref. [18], the power law in front of the exponential would be very difficult to detect experimentally since it affects the distribution for small value of  $\sigma$ .

In conclusion in this paper a frustrated Ising lattice gas has been introduced to describe different aspects of the phenomenology of granular systems, such as compaction in the presence of vibrations, logarithmic density relaxation, and exponential force distribution in agreement with real experiments. The model is able to predict new results which are amenable to experimental observation, some of which have been reported here, while others are under investigation [14]. The model which contains geometrical frustration as essential ingredient ties together features of spin glasses and glass forming liquids with those of granular materials.

Although we have reported here numerical results in 2D we expect the same features also in 3D.

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FIG. 1. Schematic picture of the lattice model considered here. Broken and continuous lines represent the two different kinds of bonds. Filled (empty) circles are present particles with spin +1 (-1).

FIG. 2. Density  $\rho(\tau, \omega_0, \epsilon_0)$  as a function of top number  $\epsilon_0$ , for top vibrations of amplitude  $\omega_0 = 0.001, 0.01, 0.05, 0.1$  (from bottom to top) and duration  $\tau = 3.28 \cdot 10^4$ . The superimposed curves are logarithmic fits from eq. (3).

FIG. 3. The density profile  $\rho(h, \tau)$  as a function of depth  $h$  ( $h = 0$  corresponds to the top of the box,  $h = 200$  to the bottom) for different values of the vibration duration  $\tau$  ( $\tau \in [3.28 \cdot 10^{-3}, 4.92 \cdot 10^4]$ ). In the bulk of the system, for fixed  $h$ ,  $\rho(h, \tau)$  is an increasing function of  $\tau$ . Continuous lines are Fermi-Dirac function fits from eq. (4). Inset: Rescaled density profile  $\rho(h, \tau)/\rho_s(\tau)$  as a function of the rescaled depth  $(h - h_0(\tau))/s(\tau)$  ( $\rho_s(\tau)$ ,  $h_0(\tau)$  and  $s(\tau)$ , are fitting parameters to obtain the data collapse).

FIG. 4. Force distribution  $F(n)$  as a function of weight  $n$  normalised by the mean force felt by the sites, for a static configuration of density  $\rho_s = 0.794$ . Superimposed is the fit function in eq. (6). The fit parameters are  $a = 12.4$ ,  $b = 5.6$  and  $c = 4.6$ . The distribution  $F(n)$  becomes narrower when the bulk density increases and is independent of the depth at which is measured (see [16]).