We introduce a lattice model, in which frustration plays a crucial role, to describe relaxation properties of granular media. We show Monte Carlo models 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 example 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 it is shaken beyond a definite threshold, the mechanical properties of sand abruptly change and the granular structure cannot be restored 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 "distancy" transition.

For a given macroscopic parameter as density a granular packing can be in a huge number of microscopic 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 [6]). In fact a characteristic of SG is their non trivial phase space which gives rise to the 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 "geometrical frustration", known also from hard sphere systems. This kind of frustration is generated by the static constraint 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 hydrodynamically frustrated system like frustrated percolation [6] and phase transitions in a granular packing have been noticed [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 degree of freedom which describes their orientation or other local structural properties of the grains. This model without gravity shows complex behavior similar to the one observed in glass forming liquids and spin glasses [6]. We will show how the density of our lattice gas is strongly dependent on the duration and the amplitude of briefly implemented vibrations. Our data reproduce the logarithmic relaxation behavior found in real experiments to 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 $\epsilon_{ii} = 1$ 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

$$\epsilon_{ij}S_iS_j = 1 \quad (1)$$

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 to 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 model consists a random diffusion of particles on a square lattice tilted by 45° (see Fig. 1) in such a way 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 $s(\gamma) = P_2(\gamma)/P_1(\gamma)$ which describes the amplitude of the vibration. It is possible to associate to this model a standard Handbook's formalism and establish a magnetic analogy,
based on the following definition:

\[-H = \sum_{\langle ij \rangle} J(\sigma_i \sigma_j S_{ij} - 1) + h_0 \sigma_i + \mu \sum_i n_i \]  

(2)

where \( S_{ij} = \pm 1 \) are spin variables, \( n_i = 0, 1 \) occupancy variables and \( \sigma_i = \pm 1 \) 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 finite temperature spin glass transition is the \( n \rightarrow \infty \) limit of the model [10], where \( S_{ij} = \pm 1 \). The mean field approach [11] was used to develop a \( T \rightarrow 0 \) limit of the model by the finite temperature version of the model [12]. In the \( T \rightarrow 0 \) limit, the spin glass is characterized by a set of \( \{ \sigma_i \} \) configurations, which are the ground states of the model [13].

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 \( \sigma_i \) on the bonds, a random initial particle configuration is prepared by randomly placing particles of given size into the box from its top and then letting them fall down, with the described dynamics (\( P_0 = 0 \), 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 overlap in the box. The system is then allowed to evolve with densities in the range \( 0.52 < \rho < 0.60 \), corresponding to a state of random loose packing.

For low densities, we have experimentally found that the system is in a state of random loose packing.

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". We have introduced "vibrations" in the interval \( t \in [0, \tau] \) linearly decreasing the ratio \( \sigma(t) \), \( \sigma(t) = \sigma_0 (1 - t/\tau) \) (with \( \sigma_0 = 1 \)).

The density \( \rho(t) \) is defined as the mean density in the lower 25% of the box (\( x_0 \) is the 0th tap number). Our results for density relaxation, in a box of size \( 30 \times 60 \) averaged over 250 different \( \{ \sigma_i \} \) configurations, are shown in Fig. 2. The behavior of \( \rho(t, \tau, \sigma_0) \) is well fitted by the following logarithmic function in agreement with the experimental data (see [11,13]):

\[ \rho(t, \tau, \sigma_0) = \rho_0 - \frac{\Delta \rho_{max}}{[1 + B \ln(t/\tau_0 + 1)]} \]  

(3)

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For \( t > \tau \) we put \( \sigma(t) = 0 \) and let the system evolve until it reaches a final "static" configuration. The final "static" bulk density \( \rho_f \) monotonically increases with the vibration time \( \tau \) asymptotically reaching a maximal density value \( \rho_f \sim 0.78 \) when \( \tau \rightarrow \infty \).

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 of 100 \( \times 200 \) and the final states have been averaged over 50 to 512 different \( \{ \sigma_i \} \) configurations (accounting the value of \( \tau \)). As suggested in Ref. [15] the density profile of granular media can be fitted using a generalized Fermi-Dirac distribution. As shown in Fig. 3 the data from our model are well fitted by such a function for different values of \( \tau \):

\[ \rho(h, \tau) = \rho_s (1 - 1/[(1 + \exp((h - h_0)/\sigma(\tau)/\sigma(\tau)))] \]  

(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]:

\[ \rho(t, \tau) = \rho_s - \rho_f \exp\left(-\left(\frac{t-t_0}{\beta T}\right)^\beta\right) \]  

(5)

Typical values of the parameters of eq. (5) in our range of \( \tau \) are \( A \in [0.15, 0.25], \beta \in [-10^4, 10^4], T \in [10^2, 10^4] \), \( t_0 \in [2, 4] \). Notice 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 density by setting \( \sigma = 1 \). Specifically, we have studied the time dependence of the particle mean square displacement \( \langle R^2(t) \rangle = \langle \frac{1}{N} \sum_i (r_i(t) - r_i(0))^2 \rangle \) of particles close to the maximal value \( \rho_f \).\( \langle R^2(t) \rangle \) shows deviations from the linear time dependence typical of standard Brownian diffusion 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 \( \langle R^2(t) \rangle \sim Dt \) we extract the diffusion coefficient \( D(\rho) \), which goes to zero at \( \rho_f \), signaling a localization transition in which particles are confined to local cages and the macroscopic diffusion-like processes are suppressed. This phenomena may also be described in a different way: \( \rho_f \) 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
The density $\rho$ coincides with the density at which the spin glass (SG) transition of Hamann-Kirkpatrick (2) is located. This implies that at $\rho$ the SG correlation length $\xi_{SG}$ diverges, signifying the presence of collective behavior in the system. In SG, this length cannot be measured 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 $w$ at the bottom follows an exponential law $P(w) = \alpha \cdot \exp(-\omega w)$. 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 an essentially scalar quantity and a crucial element is randomness in grain packing. In our later model we apply this kind of concept to study forces distributions in static configurations of the system. We suppose that each present site $w_i = 1$ 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 the right (left) neighbor has a distance $L_i$ ($L_i')$ from $w_i$, the force contribution this receives from site $w_i$ is equal to $w_i \cdot L_i / (L_i + L_i')$. We have calculated the force distribution $P(w)$ 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:

$$P(w) = \alpha \cdot \exp(-\omega w)$$  \hspace{1cm} (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 values of $w$.

In conclusion in this paper a frustrated Ising lattice gas has been introduced to describe different aspects of the phenomenology of granular systems. In agreement with experimental results which are amenable to experimental observation, some of which have been reported here, others are under investigation [19]. The model which contains geometrical frustration as an 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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[12] A static configuration is defined by the criterion that during a fixed time $t_0$, the system does not change any longer. This mean is our simulation $t_0 = 300$ time steps.

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 $\rho(r, \omega, \delta)u$ as a function of top number $\delta$, for top vibrations of amplitude $\omega = 0.001, 0.01, 0.03, 0.1$ (from bottom to top) and duration $\nu = 3.28 \times 10^7$. The supersmoothing curves are logarithmic fits from eq. (3).

FIG. 3. The density profile $\rho(h, \nu)$ as a function of depth $h$ (h = 0 corresponds to the top of the box, h = 200 in the bottom) for different values of the vibration duration $\nu$ ($\nu \in [3.28 \times 10^{-3}, 4.92 \times 10^7]$). In the bulk of the system, for fixed $h$, $\rho(h, \nu)$ is an increasing function of $\nu$. Continuous lines are fit to the data using eq. (4). Inset: Density profile $\rho(h, \nu)/\rho_0(h)$ as a function of the scaled depth $(h/\rho_0(h))/\lambda(h)$, $\rho_0(h)$ and $\lambda(h)$ are fitting parameters to obtain the data collapse.

FIG. 4. Flow distribution $F(n)$ as a function of weight $n$ normalized by the mean force felt by the sites, for a static configuration of density $\rho_0 = 0.284$. Superimposed is the fit function in eq. (6). The fit parameters are $a = 12.4$, $b = 3.8$, and $c = 4.6$. The distribution $F(n)$ becomes narrower when the bulk density increases and is independent of the depth at which it is measured (see [18]).