A THEORETICAL APPROACH TO GRANULAR MEDIA

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In connection to compaction in granular media, we describe dynamic and static properties of a lattice gas model in which frustration plays a crucial role. We show Monte Carlo results about logarithmic density increases under tapping, the Reynolds transition and exponential forces distributions. We compare moreover our findings to experimental data and try to relate the parameters in the model to experimental parameters.

1 Introduction

Relaxation processes in disordered systems, as compaction in granular media, are very often non trivial. A common and simple experiment concerns the compaction of sand. When a box filled with loose packed sand is shaken at low amplitude, the density visibly increases. The grain density compaction under tapping shows logarithmic dependence on tap number.[1] When moreover the density goes beyond a definite threshold, called the Reynolds transition, the mechanical properties of sand abruptly change and the granular structure cannot be sheared any longer without a volume increase.

A granular packing can be in a huge number of different microscopical states for each given value of macroscopic parameters as density. In order to describe this situation concepts from statistical mechanics have been introduced [2,3,4] and relations to Spin Glasses (SG) have been suggested since many years (see references in [2]). From the microscopic point of view, a crucial common aspect which appears in seemingly different materials as SG, granular media and glass-forming liquids, is the existence of mechanisms leading to frustration, as pointed out in.[6,7]

Here we describe the combined effects of vibrations and gravity in a frustrated lattice gas model introduced in,[7] in relation with some experimental facts as the compaction of sand. This microscopic model is based on an analogy with SG and frustrated percolation, which can be expressed in terms of a Hamiltonian formalism.

The model is 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 $n_i = 1$ 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: $\epsilon_{ij} S_i S_j = 1$, 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 ϵ_{ij}. As a consequence, in resemblance to frustrated percolation,[5] whenever particles close a loop in the lattice this must not be frustrated. The physical origin of the bond variables ϵ_{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 properties as grain symmetry axes.

The dynamics in our model consists in a random diffusion of particles on a square lattice tilted by 45° in such a way as to preserve the above constraint. The effects of "gravity" and "external vibrations" are introduced as follows. The particles can move upward with probability P_2 and downward with P_1 (with $P_1 + P_2 = 1$), while their spin can flip according to standard prescription to "equilibrate" local configurations, i.e. the spin flips with probability one if there is no violation of geometrical constraint, 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 is the ratio $x(t) = P_2(t)/P_1(t)$ which describes the amplitude of the vibration. This parameter fixes the final density of particles moving in a fixed volume.

The amplitude of vibrations in our model, x, and the experimental parameters of tapping may be linked more precisely. As a matter of fact, we have

$$x = \exp(-gmd/kT) \quad , \tag{1}$$

where g is the gravitational acceleration, m is the particle mass, d is the lattice spacing (of the order of particle size), and we have defined an effective temperature T (k is a dimensional constant). The case with $P_2 = 0$ (no vibrations and just gravity) described above, corresponds to $T = 0$, and the case of uniform diffusion, $P_2/P_1 = 1$, to $T = \infty$. The parameter T may be linked to an "effective temperature" of a real vibrated granular medium as described in.[2]

This model may be described in a standard Hamiltonian formalism which establishes a magnetic analogy with SG:[7]

$$-H = \sum_{<ij>} J(\epsilon_{ij} S_i S_j - 1) n_i n_j + \mu \sum_i n_i \quad . \tag{2}$$

It has been shown that Hamiltonian (2) exhibits a spin glass transition at high density.[8,10]

2 Monte Carlo results

Our system consists of a 2D box with periodic boundary conditions along the x-axis and rigid walls at its bottom and top. After fixing the random quenched ϵ_{ij} on the bonds a random initial configuration of particles is prepared by randomly pouring them into the box from the top until reaching a certain height limit.

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 with amplitude x_0 and duration τ. After each tap we have measured the bulk density of the system $\rho(t_n)$ (t_n is the n-th tap number). The behavior of our bulk density $\rho_s(t_n)$ is very well fitted by the following logarithmic function proposed to interpolate experimental data[1] (see Fig. 1):

$$\rho_s(t_n) = \rho_\infty - \Delta\rho_\infty/(1 + B\ln(t_n/\tau_0 + 1)) \quad . \tag{3}$$

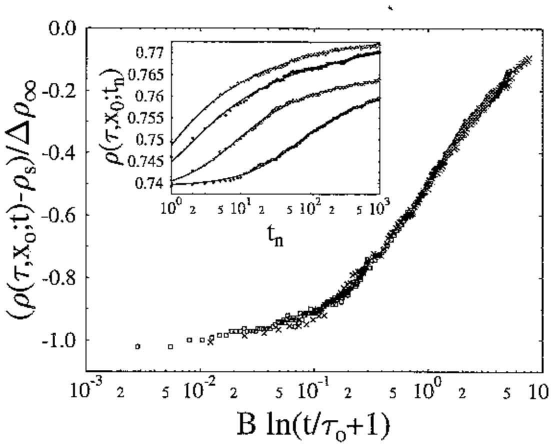

Figure 1: Experimental data from[1] (square) and our MC data (crosses) rescaled according to Eq. 3. Insert: density $\rho(\tau, x_0; t_n)$ from our MC data as a function of tap number t_n, for tap vibrations of amplitude $x_0 = 0.001, 0.01, 0.05, 0.1$ (from bottom to top) and duration $\tau = 33$. The superimposed curves are logarithmic fits from Eq. 3.

Moreover the quality of MC data allows to make predictions about the parameters in Eq. 3.[7] We find that the characteristic time in Eq. 3 is simply related to the amplitude vibration x_0:

$$\tau_0(x_0) \sim x_0^{-\gamma} \quad . \tag{4}$$

For low x_0, at fixed vibration duration $\tau = 33$ (time is measured in such a way that unity corresponds on average to a single update of each single degree of freedom), the exponent is $\gamma = 1$.

We note that this process is quite different from grain deposition after a single tap. In this second case the relaxation is of course faster, and in the long time region is well described by a "stretched exponential":

$$\rho_\tau(t) = \rho_s(\tau) - K(\tau)\ \exp[-((t - t_0)/\tau_0)^{2.3}] \quad . \tag{5}$$

The static bulk density, $\rho_s(\tau)$, depends on vibration duration τ and amplitude x_0, and increases with them, asymptotically reaching an ideal maximal density value ρ^* when $\tau \to \infty$. In our model we approximately have $\rho^* \sim 0.78$. After each tap, the deposition process leads to a static density profile, $\rho(h, \tau)$, as a function of depth h, well described by a Fermi-Dirac distribution:

$$\rho(h, \tau) = \rho_s(\tau)[1 - 1/[1 + \exp((h - h_0(\tau))/s(\tau))]] \quad . \tag{6}$$

The study, in a pure diffusive dynamics, of particle mean square displacement $R^2(t) =< \frac{1}{N}\sum_i (r_i(t) - r_i(0))^2 >$, shows deviations from Brownian motion at densities close to the maximal value ρ^*. The long time behavior of $R^2(t) \sim Dt$ defines the diffusion coefficient $D(\rho)$, which goes to zero at about ρ^*, signaling a localization transition in which particles are confined in local cages and the macroscopic

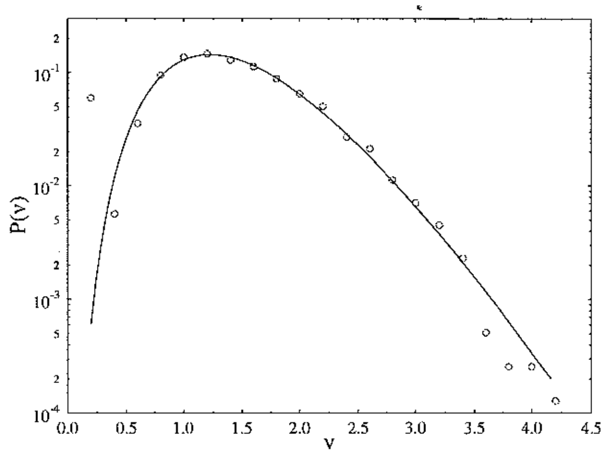

Figure 2: Force distribution $P(v)$ as a function of weight v normalized by the mean force felt by the sites, for a static configuration of density $\rho_s = 0.764$. Superimposed is the fit function in Eq. 7. The fit parameters are $a = 12.4$, $b = 5.6$ and $c = 4.6$. The distribution $P(v)$ becomes narrower when the bulk density increases and is independent of the depth at which is measured (see[11]).

diffusion-like processes are suppressed. This phenomenon seems to correspond to the quoted Reynolds transition in real granular media. The density ρ^* interestingly coincides with the spin glass transition of Hamiltonian (2). This signals the presence of a collective behavior in the system.

It is possible to introduce simplified models to describe the physics of forces in granular systems in which forces are represented by scalars.[11] In agreement with the experimental data, the broad force distribution at the bottom of our model, $P(v)$, is well fitted by an exponential corrected by a power law (see Fig. 2):

$$P(v) = a \cdot v^b \exp(-c\, v) \quad . \tag{7}$$

We find that the exponential tail is very universal, but the small forces correction depends on many details, as the geometry of the box (the distance L of its wall). Specifically when L is finite we observe that the power law reduces to a finite plateau. After a saturation region, $P(v)$ is however independent of depth h. We have also studied the dependence of $P(v)$ from the packing density. This analysis allowed to confirm some ideas of the mean field theory proposed in,[11] and to make further predictions.[7] In a silo we find that the mean force at depth h saturates according to Jannsen's law, and the force profile in horizontal planes is parabolic.

3 Conclusions

In conclusion we have discussed the properties of a frustrated Ising lattice gas, to describe some aspects of the phenomenology of granular systems. The model is strictly linked to SG and frustrated percolation. Its essential feature is the presence of frustration and the main novelty with respect to standard SG is the inclusion of particle degrees of freedom.

Introducing a very simple Monte Carlo *dynamics* in which particles diffuse and spins can flip, the model shows relaxation properties which are typical for granular media as compaction in the presence of vibrations and gravity. Subjected to tap sequences, it shows a logarithmic density relaxation corresponding to what is found in real experiments.[1] A simple model to define "forces" indicates exponentially broad force distributions as found in Ref. [11] Simulation data are in good agreement with known experimental facts and new forecasts are possible.

As predicted in Ref. [6] an interesting correspondence has emerged between the Reynolds transition in granular media and the spin glass transition of this model. This has been previously related to the structural glass transition.[8]

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