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LETTER TO THE EDITOR

The compaction in granular media and frustrated Ising models

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Abstract. 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 only 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, the 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 'dilatancy' 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 (SGs) were suggested several years ago (see references in [3]). In fact a characteristic of SGs is their non-trivial phase space which gives rise to their complex static and dynamic behaviour. The phase-space structure of SGs 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 neighbouring grains and the subsequent interlocking which leads to non-local cooperative macroscopic rearrangement. Recently, the analogies between an intrinsically frustrated system, such as frustrated percolation [6], and phase transitions in 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. This model without gravity shows complex behaviour similar to that 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 amplitude of simply implemented vibrations. Our data reproduce the logarithmic relaxation behaviour found in real experiments in a sequence of taps and offer the possibility of also making new predictions for single-tap processes. Our data also reproduce

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the distribution of forces at the bottom of the system as found in real experiments. A relation appears between the SG transition, signalled 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 $n_i = 1$ if a particle is present and 0 otherwise. The particles have an internal degree of freedom $S_i = \pm 1$, which describes the sterical properties of the grains, and are subjected to the constraint that whenever two grains (i and j) are neighbouring their 'spin' must satisfy the relation

$$\epsilon_{ij} S_i S_j = 1 \tag{1}$$

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

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. The internal variables S_i represent, for example, internal orientation of particles with non-symmetric shapes. Particles can be nearest neighbours only if the relative orientation is appropriate.

We have studied this system when subject to 'gravity' and 'external vibrations'. The dynamics of our model consists of a random diffusion of particles on a square lattice tilted by 45° (see figure 1) in such a way as to preserve the above constraint. The particles attempt a move upward with probability P_2 and a move downward with P_1 (with $P_1 + P_2 = 1$). A move is made only if the internal degrees of freedom satisfy equation (1). Similarly a spin flips with probability one if there is no violation of equation (1), and does not flip otherwise. In the 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 $x(t) = P_2(t)/P_1(t)$ which describes the amplitude of the vibration.

It is possible to associate with this model a standard Hamiltonian formalism and establish a magnetic analogy, based on the following definition,

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

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

This Hamiltonian reduces, in the $\mu \to \infty$ limit (all sites occupied), to the usual $\pm J$ *Ising spin glass* [10]. In the limit $J \to \infty$, 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. The possibility of relating the parameters of Hamiltonian (2) to definite grain properties can be based on the comparison between the behaviour of this model and actual experimental results (see [14]).

We have studied the model introduced above in a two-dimensional 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, an 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 dynamics ($P_2 = 0$), until the box is filled. To obtain an initial low-density

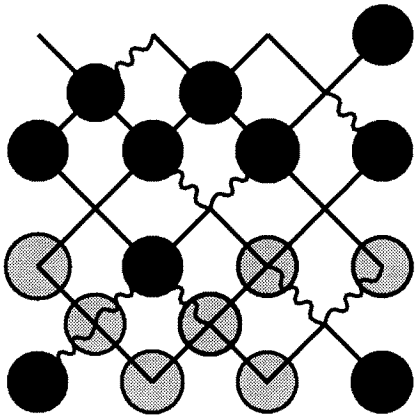

Figure 1. A schematic picture of the lattice model considered here. Wavy and straight lines represent the two different kinds of bonds ($\epsilon_{ij} = \pm 1$). Full (open) circles are present particles with spin $S_i = +1$ ($S_i = -1$).

configuration we do not allow particle spins to flip in this preparation process. The state prepared in this way has a density of about 0.520 and corresponds to 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', defined by their duration and amplitude. During a sequence of taps the density decays logarithmically to a static limit (see [11]). We have also studied this phenomena. In our MC simulation, each tap is a process in which vibrations are step like: $x(t) = x_0$ if $t \in [0, \tau]$ while for $t > \tau$ the system evolves subject only to gravity ($P_1 = 1$ and $P_2 = 0$, i.e. $x(t) = 0$) until it reaches a final 'static' configuration [12] where the simulation stops. After each tap we have measured the bulk density of the system $\rho(\tau, x_0; t_n)$ defined as the mean density in the lower 25% of the box (t_n is the nth tap number). Our results for density relaxation, in a box of size 30×60 averaged over 32 different $\{\epsilon_{ij}\}$ configurations, are shown in the insert of figure 2. The behaviour of $\rho(\tau, x_0; t_n)$ is well fitted by the following logarithmic function in agreement with the experimental data (see [11, 13]):

$$\rho(\tau, x_0; t) = \rho_s - \Delta\rho_\infty/[1 + B \ln(t/\tau_0 + 1)]. \tag{3}$$

In figure 2 we have collapsed our results for four different amplitudes as well as the experimental data for three different amplitudes on a single curve using equation (3) and see that the agreement is very satisfactory. For the data reported here, typical values of parameters in equation (3) are $\rho_s \in [0.76, 0.78]$, $\Delta\rho_\infty \in [0.02, 0.06]$, $B \in [10^{-1}, 10^1]$ and $\tau_0 \in [10^0, 10^3]$.

We have also simulated a single-tapping process. In the simulation we start at $t = 0$ from a random loose-packing configuration as described before, then we introduce 'vibrations' in the interval $t \in [0, \tau]$ linearly decreasing the ratio $x(t)$, $x(t) = x_0(1 - t/\tau)$ (with $x_0 = 1$). For $t > \tau$ we put $x(t) = 0$ 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 τ asymptotically reaching a maximal density value $\rho^* \sim 0.78$ when $\tau \to \infty$ [14].

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

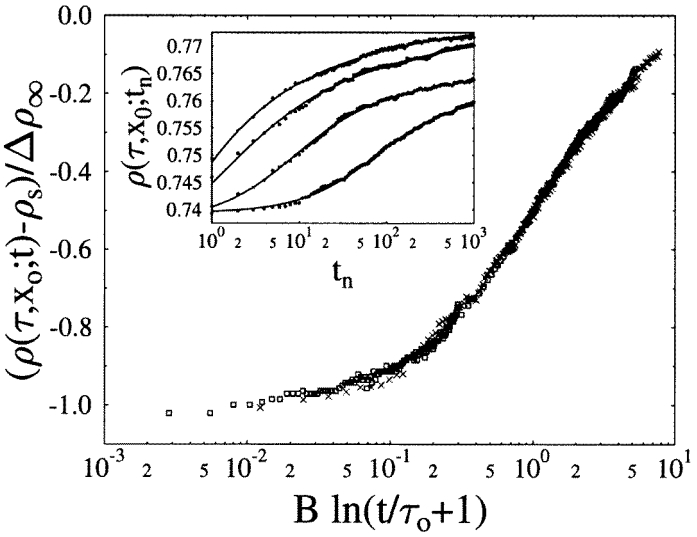

Figure 2. Experimental data from [11] (squares) and our MC data (circles) rescaled according to equation (3). Inset: density $\rho(\tau, x_0; t_n)$ from our MC data as a function of tap number t_n, for tap vibrations of amplitude $x_0 = 0.001, 0.01, 0.05, 0.1$ (from bottom to top) and duration $\tau = 3.28 \times 10^1$. The superimposed curves are logarithmic fits from equation (3).

'relaxation form' [14]:

$$\rho(t, \tau) = \rho_s(\tau) - A \exp(-((t - t_0)/T)^\beta) \tag{4}$$

Typical values of the parameters of equation (4) in our range of τ are $A \in [0.15, 0.25]$, $t_0 \in [10^0, 10^3]$, $T \in [10^2, 10^4]$, $\beta \sim 2.3$. Note that the stretched exponential behaviour only sets in after a time t_0, which can be very long if τ 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.

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

$$\rho(h, \tau) = \rho_s(\tau)[1 - 1/[1 + \exp((h - h_0(\tau))/s(\tau))]]. \tag{5}$$

The parameters in equation (5) for our data are in the range $\rho_s(\tau) \in [0.738, 0.780]$, $h_0(\tau) \in [60, 67]$ (for the box sizes given in figure 3) and $s(\tau) \in [0.4, 1.2]$.

To characterize a particle packing and its capability of internal rearrangement, we studied their self-diffusivity at fixed particle density by setting $x = 1$. Specifically we studied the time dependence of the particle mean square displacement $R^2(t) = \langle (1/N) \sum_i (r_i(t) - r_i(0))^2 \rangle$. A very interesting phenomenon is observed for densities close to the maximal value ρ^*: $R^2(t)$ 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 behaviour of $R^2(t) \sim Dt$ we extract the diffusion coefficient $D(\rho)$, which goes to zero at about ρ^*, signalling a localization transition in which particles are confined in local cages

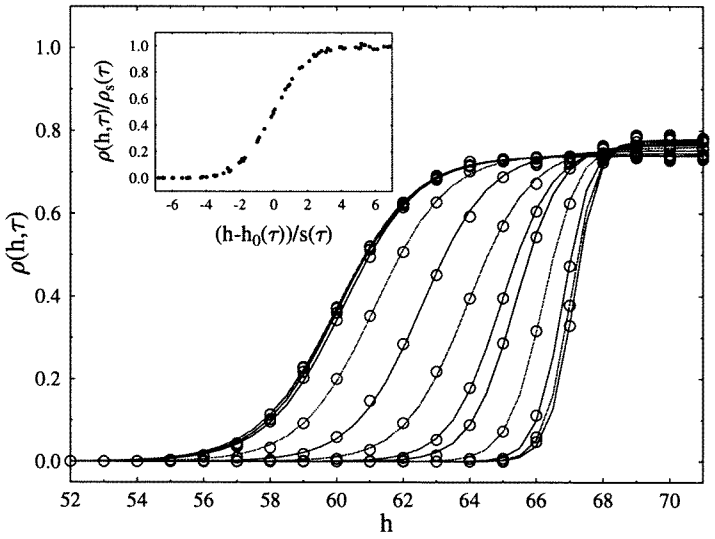

Figure 3. The density profile $\rho(h, \tau)$ as a function of depth h ($h = 0$ corresponds to the top of the box, $h = 200$ to the bottom) for different values of the vibration duration τ ($\tau \in [3.28 \times 10^{-3}, 4.92 \times 10^{4}]$). In the bulk of the system, for fixed h, $\rho(h, \tau)$ is an increasing function of τ. The continuous curves are Fermi–Dirac function fits from equation (5). 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).

and the macroscopic diffusion-like processes are suppressed. This phenomenon may also be described in a different way: ρ^* 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.

There is some evidence from other Monte Carlo simulations that the density ρ^* numerically coincides with the density at which the SG transition of Hamiltonian (2) (for $J \to \infty$) is located [8]. This should imply that at ρ^* the SG correlation length ξ_{SG} diverges, signalling the presence of a collective behaviour in the system. The coincidence of the SG transition and the suppression of self-diffusivity suggests the presence of links between the Reynolds transition in granular media, the SG transition in magnetic systems and the 'ideal' glass transition in glass forming liquids [7, 8].

The model introduced here is also suited to the study of other aspects of granular media. If a force is applied at the top of a granular system in a box, the local distribution of forces v at the bottom follows an exponential law $P(v) = a \exp(-c, v)$. As suggested in [17–19], it is possible to introduce simplified models to describe the physics of forces in granular systems. In particular, a model has been proposed in [18] in which forces are represented by scalars. In our lattice model we apply the same approximation to study the force distributions in static configurations of the system. We suppose that each present site ($n_i = 1$) carries its own weight (equal to unity) and transmits the force w_i acting on it to its first left and right neighbouring sites in the lower row. If its right (left) neighbour has a distance l_{r} (l_{l}) from site i, the force contribution it receives from this site is equal to $w_i \cdot l_{\mathrm{l}}/(l_{\mathrm{r}} + l_{\mathrm{l}})$ ($w_i \cdot l_{\mathrm{r}}/(l_{\mathrm{r}} + l_{\mathrm{l}})$, respectively, for the left site). We have calculated the force

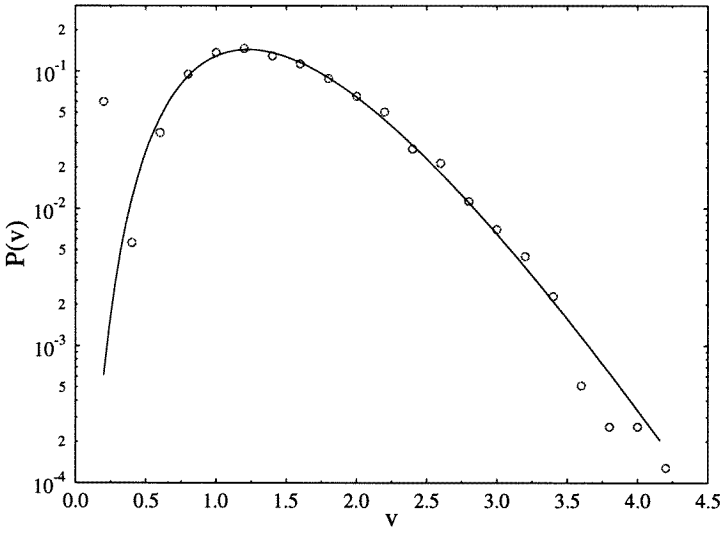

Figure 4. Force distribution $P(v)$ as a function of weight v normalized by the mean force felt by the sites, for a static configuration of density $\rho_s = 0.764$. Superimposed is the fit function in equation (6). The fit parameters are $a = 12.4$, $b = 5.6$ and $c = 4.6$. The distribution $P(v)$ becomes narrower when the bulk density increases and is independent of the depth at which it is measured (see [18]).

distribution $P(v)$ at the bottom of our system as shown in figure 4. In agreement with the experimental data and the result of the model introduced in [18], our data are well fitted by

$$P(v) = av^b \exp(-c, v). \tag{6}$$

As noted in [18], where moreover further details on the physical meaning of equation (6) may be found, the power law in front of the exponential would be very difficult to detect experimentally since it affects the distribution for small values of v. The dip present at small v originates from a pathology of our lattice model in which cavities have too regular shapes and so a large number of particles exist which carry just their own weight.

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 and an exponential force distribution. The results are in agreement with real experiments. The fact that density relaxation in this model is shown to be excellently described by the logarithmic law experimentally found is very interesting, and this suggests profound connections with the physics of granular systems. 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 an essential ingredient also shares features of spin glasses and glass-forming liquids.

Although here we have reported numerical results in two dimensions, we also expect the same features in three dimensions.

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