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► **To cite this version:**

Mario Nicodemi. Logarithmic Compaction in a 3D Model for Granular Media. Journal de Physique I, 1997, 7 (12), pp.1535-1540. 10.1051/jp1:1997154 . jpa-00247470

HAL Id: jpa-00247470

<https://hal.science/jpa-00247470v1>

Submitted on 4 Feb 2008

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Logarithmic Compaction in a 3D Model for Granular Media

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(Received 3 June 1997, revised 3 July 1997, accepted 25 August 1997)

PACS.05.40.+j – Fluctuation phenomena, random processes, and Brownian motion

PACS.46.10.+z – Mechanics of discrete systems

PACS.81.20.Ev – Powder processing: powder metallurgy, compaction, sintering, mechanical alloying, and granulation

Abstract. — We discover inverse logarithmic density compaction in a three-dimensional frustrated lattice gas subject to gravity and vibrations. The general properties of compaction are in excellent agreement with some recent experimental results with granular media and Monte Carlo simulation in two-dimensional systems.

1. Introduction

When shaken at low vibration amplitudes, dry granular media undergo an inverse logarithmic compaction [1]. One of the crucial ingredients which underlies such a slow process may be traced back to typical properties of granular assemblies as the disorder in their packing and geometric frustration felt by grains in their motion [2].

This has led to the introduction of simplified models to describe static and dynamic properties of such systems [3–6]. Lattice gas models of particles moving in a space with “quenched” disorder [7] or lattice systems of particles whose shapes induce a form of geometric frustration (not quenched) [8] have proven to exhibit an inverse logarithmic compaction when subject to gentle shaking in presence of gravity, a compaction extremely close to what is experimentally observed in granular media [1]. Interestingly these microscopic models can be cast in Hamiltonian formalism of standard Ising like systems, whose temperature plays the role of vibrations amplitude in real samples [7, 8].

The general features of these microscopic models and experimental results seems to be well described by phenomenological theories developed to explain dynamic behaviours in granular media [8–11].

Intriguing are the connections which appear with other materials where geometrical disorder and frustration play a crucial role as glassy systems [10, 12, 13]. Actually, one of the quoted microscopic lattice models [7], which we study here, without the gravitational contribution in the Hamiltonian, is a sort of diluted spin glass [14] and has been related to the physics of the glass transition in glass forming liquids [13].

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In the present paper we report for the first time about the combined effects of vibrations and gravity in such a microscopic model in three spatial dimensions. In particular we analyse grains density relaxation during shaking and relate Monte Carlo (MC) observations to corresponding phenomena in real experiments. In spite of the schematic Monte Carlo diffusive like dynamic here used, we recover the inverse logarithmic behaviour known from experimental measurements in sequences of taps [1]. The robustness to changes of this structural property suggests its universality and support the quoted phenomenological theories.

2. The Model

We consider a three-dimensional version of the model introduced in [7], a system of particles diffusing on a body centered cubic lattice whose edges between neighboring vertexes are characterized by quenched random numbers $\epsilon_{ij} = \pm 1$. As in usual lattice gases, to each site i of the lattice we associate an occupancy variable $n_i = 0, 1$ indicating the absence or presence of a particle. Moreover particles are characterized by an internal degree of freedom described by an Ising variable, $S_i = \pm 1$, which schematically indicates their orientation (for instance horizontal or vertical). In the complex dynamical characteristic processes of real granular media, grains are typically frustrated in their motion by several microscopic mechanisms as, for instance, geometrical effects due to hard core repulsion with their neighbours or friction phenomena. These effects are schematically introduced in the present model by requiring that particles cannot overlap and moreover that their orientations, S_i , have to match the local geometrical environment. To this aim we impose that whenever two (i and j) are neighboring, their “spin” must satisfy the relation $\epsilon_{ij} S_i S_j = 1$. Thus, in our picture, the quenched edges variables, ϵ_{ij} , are introduced to schematically take into account the typical local effects leading to frustration in real samples, disregarding the actual mechanisms from which it arises. Let’s notice that at high enough density, the effects of the “quenched” disorder are apparent, because, as in frustrated percolation [15], particles cannot close frustrated loops (see [7, 14, 15]). Thus the maximal density will typically be well inferior to one.

If in our system “gravity” would play no role, as in glassy systems, the simplest dynamics would be a usual random diffusion of particles in the lattice, with the possibility of spin flip (if the above constraints are satisfied). In presence of gravity and “external vibrations”, diffusion is no longer isotropic. Thus in our model, particles attempt a move upward with probability P_2 and downward with P_1 , with $P_1 + P_2 = 1$. When vibrations are off, the presence of gravity imposes $P_2 = 0$, however, when vibrations are switched on, P_2 becomes finite ($P_2 \leq P_1$). The crucial parameter for the dynamics in our model is the ratio $x(t) = P_2(t)/P_1(t)$ which describes amplitude and duration of “vibrations” in our Monte Carlo.

We refer to the papers quoted in [7] to elucidate the mapping into Ising Spin Glasses and the relation between the parameter x and the temperature of the magnetic equivalent system.

As stated above, in our Monte Carlo simulations we consider a body centered cubic lattice with periodic boundary conditions along the horizontal axis (respect to gravity) and rigid walls at bottom and top. The edges of the lattice are given the random quenched values ϵ_{ij} . The particles are randomly inserted from the top and deposited with the described dynamics towards the bottom (by the moment $P_2 = 0$), until the box is filled. The two basic Monte Carlo moves (the spin flip and particle hopping) are done in random order.

3. Simulations of Sequences of Taps

In real experiments on compaction in granular media, the density relaxation is observed during sequences of taps, where a “tap” is the shaking of a filled container using vibrations

of given duration and amplitude. In our MC simulations (see Ref. [7] for further information), each single tap is schematically represented with the diffusive dynamics described above: the particles in the lattice move around with probabilities P_1 and P_2 whose ratio is kept constant $x(t) = x_0$ for $t \in [0, \tau]$ and then is set to zero (only gravity) for a time long enough. If during a fixed time t_0 nothing changes in the system, we consider that it has attained a static configuration. This “shaking” procedure is repeated for a given number of taps (in our case 250). In the following simulations, we have chosen $t_0 = 1300$, much longer than any intrinsic time in absence of vibration, and, actually we observed no changes during t_0 (time is measured in such a way that one unit corresponds to one single average update of all particles and all spins in the lattice). In our simulations, by definition τ is the duration of the vibrations of a tap and x_0 the amplitude.

To observe compaction, the quantity we are interested in is the static bulk density of the system, $\rho(t_n)$, defined as the average density in the lower 25% of the box measured after each tap (t_n is the n -th tap number). We selected this quantity to make explicit the confrontation with experiments as in reference [1]. However it is worth to notice that the same behaviour is recorded for the densities of the upper regions of the bulk of the system. In our Monte Carlo experiment we considered several tapping sequences for different values of the tap amplitude x_0 and fixed duration τ (we took $\tau = 40$). The length of the sequences is fixed to 250 taps, averaged over 32 different $\epsilon_{i,j}$ configurations.

We deal with a box whose horizontal surface is 8×8 and height of 24 lattice spacing units. This kind of simulations require long CPU times, and this fixes the limit for the sizes of the system. However we checked that our general results are independent on finite size effects.

As stated, experimental data about grain density compaction during a sequence of taps are well interpolated by an inverse logarithmic law [1]. Writing in explicit form the asymptotic variation in density as the difference of a final asymptotic value (ρ_∞) and an initial value (ρ_0), such a law can be cast in the following form:

$$\frac{\rho(t_n) - \rho_\infty}{\rho_0 - \rho_\infty} = \frac{\ln(c)}{\ln(t_n/\tau_0 + c)} \quad (1)$$

where c and τ_0 are parameters. Monte Carlo data about density relaxation under tapping of a two-dimensional version of the present model have proved satisfy very well equation (1) and were excellently rescaled with experimental data [7].

Our data for the present three-dimensional system show surprising agreement with the findings in two dimensions. Density compaction during the sequences of our MC taps of fixed duration τ and amplitude x_0 , is well interpolated with equation (1). Moreover, in precise correspondence with the 2D system, the parameter $c = 1.3$ (this is the same numerical value found in 2D) may be considered as almost independent of x_0 in the range explored $x_0 \in [5.0 \times 10^{-3}, 0.5]$ (we work at fixed τ). We impose that the fit function for density data passes at $t_n = 0$ in $\rho_0 = 0.5552$, *i.e.*, the measured average static initial state density of the system, and thus the parameters of the fit with equation (1) are reduced to just two. Thus we deal with reasonably controllable quantities.

In Figure 1 we report MC data about density compaction. The superimposed fits are with the inverse logarithm of equation (1), and the values of the two fitting parameters ρ_∞ and τ_0 are shown in Figure 2. The quality of the fit is very good and one could collapse both MC data in two and three dimensions and experimental data on a single master curve as in reference [7].

The parameter τ_0 approximately follows a power law as a function of the vibration amplitude x_0 (at fixed $\tau = 40$):

$$\tau_0(x_0) = (x_0/X)^{-\gamma} \quad (2)$$

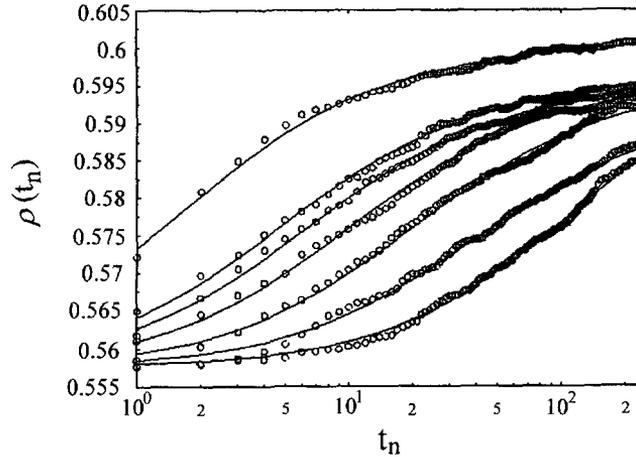


Fig. 1. — Static bulk density $\rho(t_n)$ from our MC data in a body centered cubic lattice as a function of tap number t_n , for tap vibrations of amplitude $x_0 = 5.0 \times 10^{-3}, 1.0 \times 10^{-2}, 2.0 \times 10^{-2}, 5.0 \times 10^{-2}, 7.0 \times 10^{-2}, 0.1, 0.5$ (from bottom to top) and duration $\tau = 4.0 \times 10^1$. The continuous curves are logarithmic fits from equation (1), the parameters of which are given in Figure 2. Such a logarithmic interpolation has been proposed to fit experimental data (see Ref. [1]) and was found in simulations of two-dimensional systems too.

For low values of the “vibrations amplitude”, x_0 , of our Monte Carlo, the exponent is $\gamma \simeq 1.0$ and $X = 1.45$ (see Fig. 2). This result has a direct correspondence with the findings from simulations in two spatial dimensions in system with both “quenched” disorder as the present [7] and with no quenched disorder [8]. Actually also in these apparently different cases the exponent γ is close to one. The parameter x_0 may be related to the effective temperature of our lattice gas as explained in reference [7]. A granular effective temperature may be also introduced in real granular media, as described for instance in [2], as a function of the amplitude and frequency of vibrations of real experiments. The confrontation of these temperatures may suggest a way to relate x_0 to measurable quantities and to a direct experimental investigation of equation (2).

A crude approximate fit to link ρ_∞ to x_0 for intermediate values of x_0 is (as in 2D):

$$\rho_\infty(x_0) = r_1 + r_2 \ln(x_0) \quad (3)$$

with $r_1 = 0.60$ and $r_2 = 0.002$ (see Fig. 2).

Equation (1) has a phenomenological origin to fit experimental data, and might be actually substituted by other analogous functional form. However, it is interestingly in general agreement with some phenomenological theories introduced to describe density compaction in granular media from simple geometrical arguments [8–11]. Our finding about different systems with different dimensionality supports the validity of the arguments from such theories. At the same time, our detailed results about the parameters of equation (1) (see Eqs. (2, 3)) offer possible probes for such theories.

4. Conclusions

In conclusion, we have studied a three-dimensional frustrated lattice gas, related to spin glasses and to frustrated percolation, which shows an inverse logarithmic density compaction, under

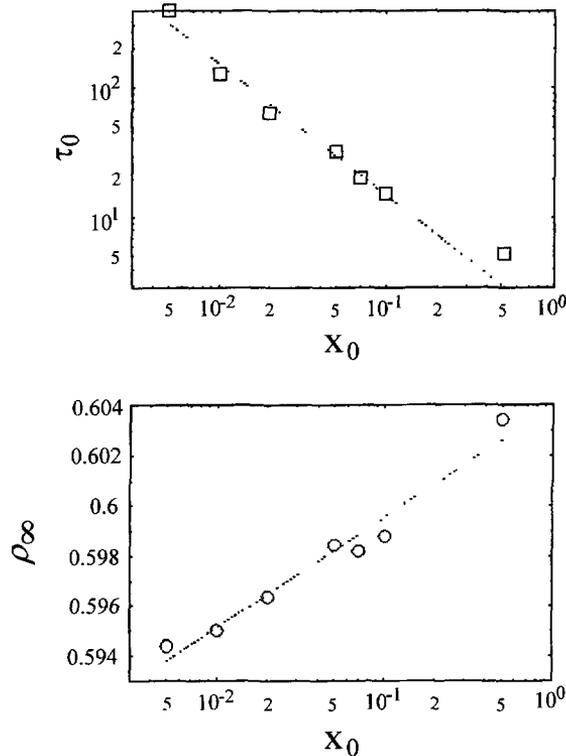


Fig. 2. — Fit parameters ρ_∞ and τ_0 for density relaxation from equation (1), as a function of vibration amplitude x_0 . The superimposed curve on $\tau_0(x_0)$ is a fit with a simple power law: $\tau_0(x_0) \sim x_0^{-\gamma}$. The exponent $\gamma \sim 1.0$ has a value close to what is numerically found in two-dimensional systems.

gentle shaking, extremely close to the behaviour found in real experiments on granular media [1].

The logarithmic behaviour in density compaction is actually observed in very different models with [7] or without [8] quenched disorder and in both two and three spatial dimensions. A common crucial element, from the microscopic point of view, present in these different lattice models is a sort of “frustration” felt by particles in their motion under gravity and vibrations. Interesting is also the finding that parameters, as τ_0 , of such logarithmic relaxation show a power law behaviour with the schematic vibration amplitude x_0 of our Monte Carlo dynamic, power law which is close in all these different models. These results from the more controllable Monte Carlo experiments should stimulate further experimental investigations. They support moreover the approach of general phenomenological theories recently introduced to explain slow compaction processes in granular media [8–11] and offer a possibility for their probe.

The same model we studied here, in absence of gravity, has been related to the physics of the glass transition in glass forming liquids [13].

Acknowledgments

It is a pleasure to thank Hans J. Herrmann and Antonio Coniglio for our interesting discussions. Moreover I thank IDRIS for computer time on Cray-T3D, and the “Universita di Napoli Federico II” and the “Fondazione A. Della Riccia” for financial support.

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