A minimal model for slow dynamics: Compaction of granular media under vibration or shear

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Abstract: Based on experiments of the compaction of granular materials under periodic shear of a packing of glass beads, a minimal model for the dynamics of the packing density as a function of time is proposed. First, a random "energy landscape" is created by a random walk (RW) in energy. Second, an ensemble of RWs is performed for various temperatures in different temperature-time sequences. We identify the minimum (mean) of the energy landscape with the maximum (random) density. The temperature scaled by the step-size of the energy landscape determines the dynamics of the system and can be regarded as the agitation or shear amplitude. The model reproduces qualitatively both tapping and shear experiments.

Key-words: Compaction, crystallization, Sinai-diffusion, random walks, quenched disorder

1 Introduction

The issue of slow dynamics, rare events and anomalous diffusion is object to ongoing research in statistical physics [4, 7, 13, 21, 22]. One example for an experimental realization of slow dynamics is the compaction of granular materials, being of interest for both industrial applications and research. Many compaction experiments have been carried out in the last decades, see e.g. [1, 2, 6, 12], but the evolution of density with time is far from being well understood. Recent laboratory experiments concern pipes filled with granular media and periodically accelerated in order to allow for some reorganization [9, 17, 18]. The compaction dynamics was obtained to be logarithmically slow and could be reproduced with a simple parking model [3, 11]. Alternative experiments concern a sheared block of a granular model material (monodisperse glass spheres) and display a similar dynamics [16]. Numerical model approaches, like a frustrated lattice gas (the so-called "Tetris" model) [5, 15, 20] also lead to this slow dynamic behavior, as well as some theory based on stochastic dynamics [14]. The fact that a peculiar dynamics is reproduced by so many models indicates that it is a basic and essential phenomenon.

Rather than modeling granular systems in all details, e.g. in the framework of molecular dynamics or lattice gas simulations [19, 20], we will propose a very simple model based on the picture of a random walk in a random energy landscape, for a review see [4], and even simpler than recent, very detailed considerations in the same spirit [8]. Random walks have been examined, for example, on fractals and ultrametric spaces, where the continuous time random walk was introduced in order to allow a mathematical treatment [10]. If a random walker is situated in a uncorrelated, random, fractal energy landscape, the process is called Sinai-diffusion [4]. The aim of this study is to show that the Sinai model is in qualitative agreement with the compaction dynamics of granular media. An issue not addressed here is a quantitative adjustment which can be reached, for example, by introducing correlations in the EL.

2 Summary of the experimental results

The subject of compaction of granular material [1, 2, 6, 12] has been recently revisited through careful experiments carried out by Knight et al. and Nowak et al. [9, 17, 18]. The experiment consists of a vertical cylinder, full of monodisperse beads, which is submitted to successive distinct taps of controlled acceleration (vertical vibration). The measurement of the mean volume fraction after each tap gives a precise information about the evolution of the compaction. From the first experiments performed with taps of constant amplitude, the increase in volume fraction was found to be a very slow process well fitted by the inverse of a logarithm of the number of taps. Nowak et al. [17, 18] have then studied the compaction under taps of variable amplitude, and showed that irreversible processes occur during the compaction. Starting with a loose packing, the evolution of the volume fraction is not the same when increasing the amplitude of vibration as when decreasing. The first branch appears to be irreversible, whereas the second is reversible.

We have recently performed a compaction experiment based on cyclic shear applied to an initially loose granular packing [16]. A parallelepipedic box full of beads is submitted to a horizontal shear through the periodic motion of two parallel walls at amplitude $\theta_{\max}$, see Fig. 1(a). Compaction occurs during this process, leading to crystallisation of the beads in the case of a monodisperse material. The control parameter in this configuration is the maximum amplitude of shear $\theta_{\max}$ (inclination angle of the walls). The measurement of the mean volume fraction ϕ shows that compaction under cyclic shear is a very slow process as in the vertical vibration experiments (typically 5×10^4 shear cycles or taps). The higher the shear amplitude the more efficient is the compaction (shear amplitudes up to $\theta_{\max} < 12.5^\circ$ were examined), when starting with a loose packing of the same initial volume fraction. More surprising results arise when the packing is submitted to a sudden change in shear amplitude. We have observed that a "jump" in volume fraction occurs which is opposite and proportional to the change in $\theta_{\max}$. Sudden increase (resp. decrease)

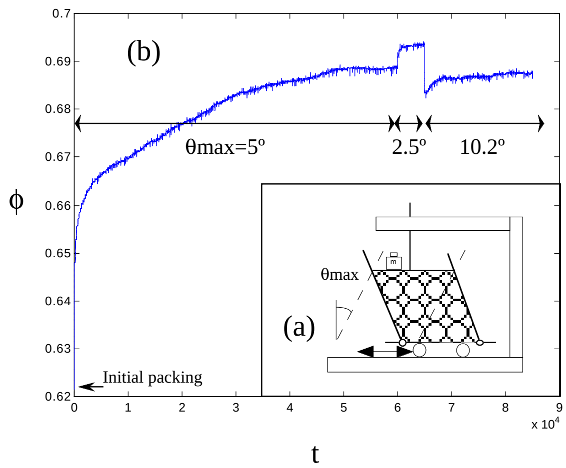

Figure 1: (a) Sketch of the experimental setup. (b) Evolution of the volume fraction as function of shear cycles n: a saturated state is seemingly reached after 6×10^4 cycles with an initial shear angle of 5 degrees; a positive jump in volume fraction is observed when the angle is decreased to 2.5 degrees and applied for 5×10^3 cycles; a negative jump is observed when the angle is increased to 10.2 degrees.

in the shear amplitude decreases (resp. increases) the volume fraction (Fig. 1). The response is very rapid (less than 20 cycles) and quasi-independent of the state before the angle change. For more detailed experimental results see [16].

3 The Model

A naive picture that evolves out from the experimental observations is the analogy between the packing of beads and a thermal system seeking for a minimum of energy in a very complex potential-energy landscape [4]. Due to some agitation (shear) compaction occurs and the total potential energy of the packing decreases. Starting from a loose packing at $n = 0$, the vibrational or shear excitation can be seen as the analog of the temperature in the sense that the excitation allows for an exploration of the phase space. In a granular packing of monodisperse spheres, the absolute minimum of the energy is obtained for a perfect (fcc) or (hc) crystal with volume fraction $\phi = 0.74$. If the energy landscape is complex with a lot of different scale valleys or hills, one can understand that an efficient, fast compaction will be obtained with high temperatures: the system is then able to escape the deep local valleys and find a valley with lower potential energy. A decrease of the temperature is then needed to explore local fine-scale minima. The goal of this paper is simply to explore this idea by studying the dynamics of random walkers on a random landscape (the Sinai model), and to show that this very naive picture gives results in qualitative agreement with the experimental observations.

Our model is based on the assumption that all possible configurations of a granulate in a given geometry can be mapped onto an "energy landscape" (EL). Since a simple two-level system (as used to model the dynamics in simple glasses) does not lead to the experimentally observed phenomenology, we assume a fractal energy landscape created by a random walk in energy with phase space coordinate x. A typical EL with energy $V(x)$ is schematically shown in Fig. 2. The stepsize in energy is ΔV, the mean of the energy landscape is $V_{\rm mean}$ and its absolute minimum is $V_{\rm min}$. Here, the EL is symmetric to its center, in order to allow for periodic boundary conditions in x. Given some EL, the granulate is now modeled as an ensemble of random walkers diffusing on the EL, with a temperature T_{RW}. The analog to the density of a granular packing is the rescaled energy of an ensemble of random walkers in the energy landscape

$$\nu = 1 - \frac{E - V_{\rm min}}{V_{\rm mean} - V_{\rm min}} \ , \tag{1}$$

which we denote as *density* in the following. For the (random) initial configuration, the energy will be $E \approx V_{\rm mean}$ so that $\nu = 0$; for the close-packing configuration, i.e. all RWs are in the absolute minimum, one has $E \approx V_{\rm min}$ and thus $\nu = 1$. The energy landscape has the size L, the ensemble of RWs consists of R random walkers and S is the number of steps performed.

Since the energy of the RWs in the EL corresponds to the potential energy of the packing, we interpret the (constant) stepsize ΔV (used here as one possibility for the construction of the EL) as a typical activation energy barrier. The maximum of V corresponds to a random loose, local packing density, the mean to the (initial) random close packing, and the absolute minimum to the hexagonal close packing. For one RW, the probability to jump within time Δt from one site x_i to its neighbor-site $x_{i\pm1}$ is

$$p_\pm(x_i) = \min\left[1, \exp(-\Delta_\pm(x_i)/T_{RW})\right] \ , \tag{2}$$

with $\Delta_\pm(x_i) = V(x_{i\pm1}) - V(x_i)$. Since ΔV is the only energy scale of the system, we define the dimensionless energy steps $\delta^i_\pm = \Delta_\pm(x_i)/\Delta V$ and the dimensionless temperature $T = T_{RW}/\Delta V$. Written in dimensionless parameters, the jump probabilities are thus $p^i_\pm = p_\pm(x_i) = \min\left[1, \exp(-\delta^i_\pm/T)\right]$, so that a particle always jumps downhill ($\delta^i_\pm \le 0$), but jumps uphill only with a probability $e_0 = \exp(-1/T)$ (for $\delta^i_\pm > 0$), at finite temperature. The limits $T \to 0$ and $T \to \infty$ correspond thus to immobile particles or to a homogeneous RW, respectively. The discrete master equation for the probability density $n^i(t)$, to find a particle at time t at site i of the

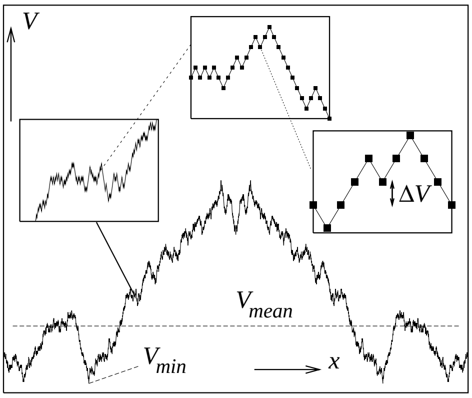

Figure 2: Schematic plot of a typical energy landscape as used for the simulations. The insets show different zoom levels, in order to get an idea of the local situation. For an explanation of the symbols, see the text.

EL, is

$$n^i(t+\Delta t) - n^i(t) = -\left[p_+^i + p_-^i\right] n^i(t) + p_-^{i+1} n^{i+1}(t) + p_+^{i-1} n^{i-1}(t) \quad (3)$$

and is (straightforwardly) simulated with $R = 200$ random walkers in an energy landscape with $L = 5000$ sites, if not explicitly mentioned. The time interval Δt corresponds to one Monte-Carlo step but *not* to one shear-cycle n. For the sake of simplicity, we measure x in units of the distance between neighboring sites $\Delta x = x_{i+1} - x_i = 1$, and time in units of Δt. The diffusion constant of a homogeneous random walk ($p_\pm = 1/2$ or $T \to \infty$) is thus $D = \Delta x^2/\Delta t = 1$. For a constant occupation probability (initial density $n_c = n^i(t=0) = R/L = \mathrm{const.}$), one can extract the diffusion constant D_c as function of the temperature, since $p_\pm = 1/2$ and $p_\pm = e_0/2$ occur with equal probability, so that

$$D_c(T) = \frac{1+e_0}{2} = \frac{1+\exp(-1/T)}{2} \; . \quad (4)$$

In Fig. 3, $D_c = R_2(t)/\sqrt{t}$ is plotted against T after different times t, with $R_2(t) = \langle (x(t) - x_0)^2 \rangle$. For large T, the system does not feel the EL and behaves like an ensemble of homogeneous RWs, whereas its behavior becomes subdiffusive after several steps for small T when the EL is explored. In a situation with $T \approx 0$, after a rather short transient, all RW will occupy a local minimum, a valley ($\vee$), wheras the unstable local configurations hill ($\wedge$), or left- (/) and right-slope (\) cannot be occupied. if T is small enough, the random walkers stay trapped. Note that this statement is strictly true for $T = 0$ or when a fixed number of shear-cycles or taps is implied. In the Sinai diffusion model, for a finite system, the RW will always find

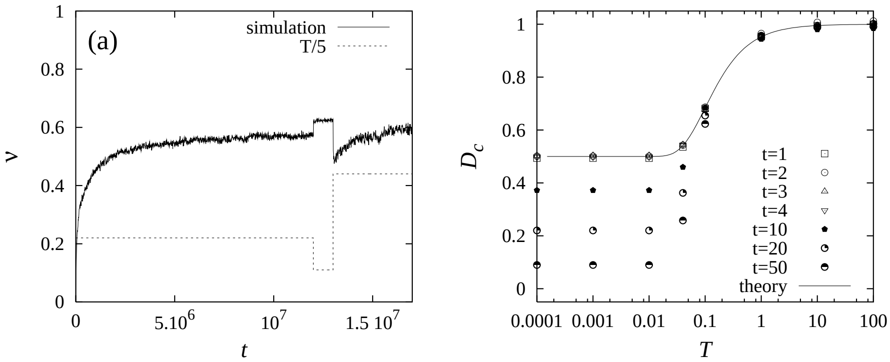

Figure 3: (a) Density plotted against time t (in units of Monte-Carlo steps) for a simulation with $T_0 = 1.1$, $L = 5000$ and $R = 200$. The temperature-sequence is indicated by the dashed line. (b) Diffusion constant $D_c = R_2(t)/\sqrt{t}$ at time t as function of temperature T for systems with constant (initial) density. The solid line shows Eq. (4).

the global minimum – the temperature only determines the time-scale of this process [4]. Since the duration of an experiment is limited, the global minimum cannot be found by all particles if the phase space volume L is large enough.

4 Results and Discussion

In parallel to the tapping experiments by Nowak et al. [18], we present simulations of our model using a periodic time series for the temperature. The temperature is kept constant for S steps and then increased by $\Delta T = 0.1$, where it is kept again constant for S steps. T is initially zero and then raised up to $T = 2$. From this state, T is decreased to zero and the loop is repeated seven times. In Fig. 4, the simulation results are displayed for different S as given in the inset. In the initial branch with increasing T, the density increases and slowly decreases for large T. This branch is irreversible, but the periodic loops show almost reversible behavior. For very short loops (small S), the density continuously increases, for longer loops the behavior of the system is reversible. Note that the system also shows hysteretic behavior, the density at decreasing T is below the density at increasing T.

In summary, we presented a very simple model for the dynamics of the compaction of granular media due to an external agitation. Our model is not as detailed as others (parking lot or frustrated lattice-gas models), but it is extremely simple and still shows qualitative agreement with two different types of experiment. Its simplicity allows for future analytical treatments. However, such a simple model arises, besides

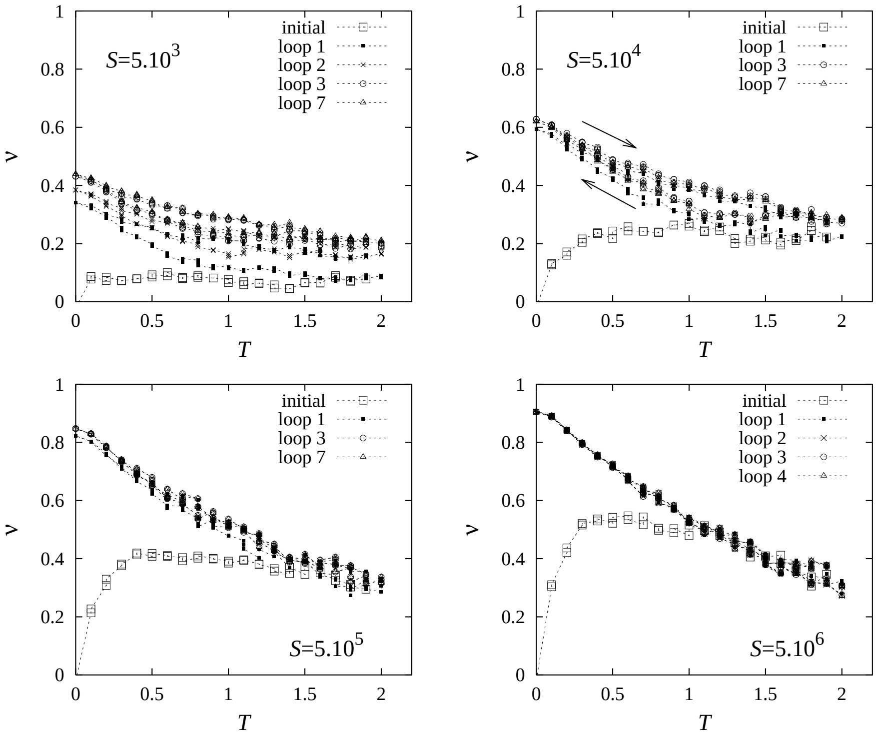

Figure 4: Rescaled density ν plotted as a function of the temperature T for a periodic temperature sequence. The arrows indicate the direction of the loops.

many others, two major questions: (i) Is it possible to link the real configuration phase space with the an energy landscape? (ii) Is it correct to do the analogy between the experimental external excitations like shear or tapping with a temperature?

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