

A “Tetris-Like” Model for the Compaction of Dry Granular Media

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We propose a two-dimensional geometrical model, based on the concept of geometrical frustration, conceived for the study of compaction in granular media. The dynamics exhibits an interesting inverse logarithmic law that is well known from real experiments. Moreover, we present a simple dynamical model of N planes exchanging particles with excluded volume problems, which allows us to clarify the origin of the logarithmic relaxations and the stationary density distribution. A simple mapping allows us to cast this Tetris-like model in the form of an Ising-like spin system with vacancies. [S0031-9007(97)03818-0]

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A granular system may be in a number of different microscopic states at fixed macroscopic densities, and many unusual properties are linked to its nontrivial packing [1,2]. As pointed out by Edwards [2–4] the role that the concept of free energy plays in standard thermal systems as Ising models, in granular media seems to be played by the “effective volume,” derived by a complex function of grain positions and orientations. In this way statistical mechanics provides theoretical concepts in the context of nonthermal systems.

A recent experiment on the problem of density compaction in a dry granular system under tapping has shown [5] that density compaction follows an inverse logarithmic law with the tapping number.

Several approaches have been proposed to explain this behavior [6–11], as geometrical models of “parking” [10,12] or simple free-volume theories [11] or the study of the dynamics of a frustrated lattice gas with quenched disorder subject to gravity and vibrations [9].

In many seemingly different cases the logarithmic relaxation proposed in [5] to describe experimental data is reproduced. Moreover, the logarithmic law has turned out to be robust with respect to changes in the tapping procedure [9]. This suggests that such a relaxation behavior is extremely general and not linked to specific properties of definite realizations.

Here we introduce a purely geometrical model of simple particles with several shapes on a lattice. We show that when subject to gravity and vibrations a logarithmic density relaxation [5] is found, due to the high entropic barriers (originated for geometrical reasons) to be passed by particles to improve global packing.

We imagine a model similar to the computer game *Tetris*, in which neighboring grains can find different packing volumes according to their relative geometrical orientations. Although one could imagine a rich variety of

shapes and dimensions, as in the real computer game, it is useful, without loss of generality for the main features, to think just of a system of elongated particles which occupy the sites of square lattice tilted by 45° (see Fig. 1, with periodic boundary conditions in the horizontal direction (cylindrical geometry) and a rigid plane at its bottom. In general, the only interactions between the particles are the geometrical ones. Particles cannot overlap, and this condition produces very strong constraints (frustration)

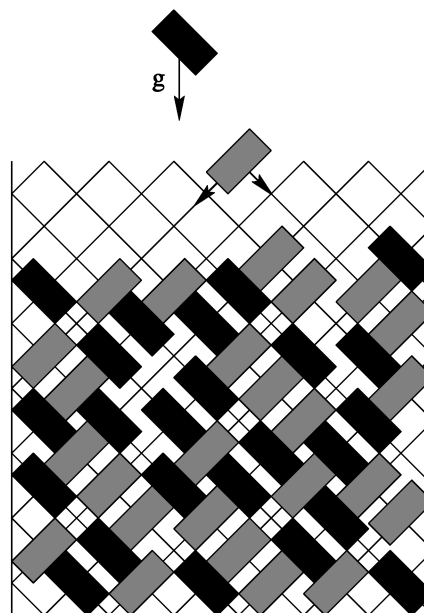


FIG. 1. Schematic picture of one particular configuration of the grains considered in the simplest version of the Tetris-like model. The two types of particles have to fulfill only geometrical constraints in their dynamics. As shown in the figure these constraints are due to the impossibility for the particles to overlap.

on their relative positions. For instance, in the simplest case of two kinds of elongated particles pointing in two (orthogonal) directions, the frustration implies that two identical particles (pointing in the same direction) cannot occupy neighboring sites in this direction. The particles are in principle allowed to rotate if at least three of their nearest neighbors are empty. This condition is such that for sufficiently high densities the rotation events become negligible and the particles keep definitely their orientation. It is then reasonable, in the limit of a sufficiently large system, to consider an equal number of the two kinds of particles. There is no other form of interaction between particles, and in this sense the model is purely geometrical.

As stated, the particles are confined to a box and subjected to gravity. The effect of vibrations is introduced by allowing the possibility of also moving upwards, as explained below.

The system is initialized by filling the container. The procedure of filling consists of inserting the grains at the top of the system, one at the time, and letting them fall down, performing, under the effect of gravity, an oriented random walk on the lattice, until they reach a stable position, say a position in which they cannot fall further. This filling procedure is realized by the addition of one particle at a time and stops when no particles can enter the box from the top anymore.

In our case the dynamics can be divided in two alternating steps. First, in a *heating* process (tapping) the system is perturbed by allowing the grains to move in any allowed directions with a probability p_{up} to move upwards (with $0 < p_{\text{up}} < 0.5$) and a probability $p_{\text{down}} = 1 - p_{\text{up}}$ to move downwards. After each tapping has been completed (i.e., a fixed number N moves per particle have been attempted with a fixed value of $x = p_{\text{up}}/p_{\text{down}}$), we allow the system to relax setting $p_{\text{up}} = 0$. The relaxation process (*cooling*) is supposed to be completed just when no particles can move anymore under just the effect of gravity, i.e., unless p_{up} is switched on. After this relaxation the system is in a stable static state and one starts again the cycle. We verified how the basic features of our model are very robust with respect to variations in the Monte Carlo procedure. It is worthwhile to stress how our dynamical procedure is very close physically to the real processes of vibro-compaction [13]. Work is in progress to implement in our system the method proposed in [14] which allows for the simulation of a real tapping process.

More precisely, the single dynamical step consists of the following operations: (1) extracting a grain with uniform probability; (2) extracting a possible movement for this grain among the four first neighbors (two for the cooling process) according to the probabilities p_{up} and p_{down} ; (3) moving the grain if *all* the possible geometrical constraints with the neighbors are satisfied.

We performed numerical simulations of the Tetris-like model in order to investigate its compaction properties.

In particular, we measured the density of the packing, i.e., the percentage of sites occupied with respect to the total number of sites, after each relaxation step and, in correspondence with real experiments, we plot the behavior of this density as a function of the number of taps. In order to avoid finite-size effects we considered systems with a linear size of at least $L = 50$ sites and, in order to be sure to observe bulk effects, we measured the density in the lower 25% of the system.

Our main results on compaction are summarized in Fig. 2 which shows the evolution of the density, as a function of the number of taps, for different values of x and for a system of dimension $L = 50$. The different curves, obtained with a tap length of one iteration per particle, can be fitted according to the following inverse logarithmic law:

$$\rho(t_n) = \rho_\infty - \frac{\Delta\rho_\infty}{1 + B\ln(t_n/\tau + 1)}, \quad (1)$$

with $\rho_\infty = 1$, a value $\Delta\rho_\infty = 0.25$, which depends only on the loose packing density $\rho_{t_0} \sim 0.75$, and two free parameters, B and a characteristic time τ , for which we observe an algebraic dependence on x :

$$\tau = Ax^{-\gamma}, \quad (2)$$

where $\gamma \simeq 0.84$ and $A = 4.3$. In this case τ has the meaning of the minimum time over which one starts to observe a compaction process. Up to times $t_n \ll \tau$, in fact, $\rho(t_n)$ keeps practically the initial value. A complete and detailed analysis of these numerical results is reported in [15].

Let us now briefly discuss how the system reaches the close-packing density which, just in the case of the simplest version with only two possible shapes, corresponds

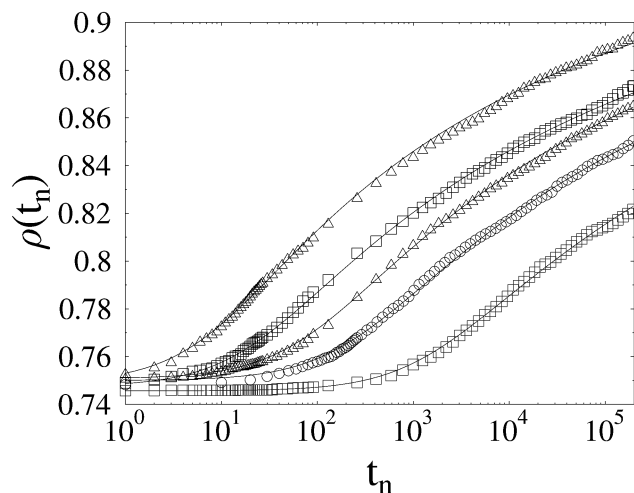


FIG. 2. Logarithmic behavior of the density of the packing, measured in the lower 25% of the system, as a function of tapping number t_n , for five different values of amplitude vibrations $x = p_{\text{up}}/p_{\text{down}} = 0.001, 0.01, 0.03, 0.1, 0.5$, from bottom to top. The superimposed logarithmic fit curves, given by Eq. (1), were proposed to describe experimental data.

to a perfectly ordered state with unitary density. It is worth stressing again how this choice does not change the qualitative behavior of the system, and an infinity of disordered ground states can be obtained just allowing for a rich variety of shapes for the particles [15]. The approach to this state, realized by means of the two-step dynamics described above, represents a complex nonequilibrium process in which the system evolves alternatively with two different “temperatures:” a temperature T_2 (heating process) such that $e^{-2g/T_2} = \frac{p_{\text{up}}}{1-p_{\text{up}}}$ and a temperature $T_1 = 0$ for the cooling process. The first step could be considered as a process going towards equilibrium in which detailed balance holds. Its features in many respects are very similar to the simple *hard-square model* [16]. The step at zero temperature is an out of equilibrium process which involves an irreversible positioning of the particles. Globally the microscopic reversibility and detailed balance are lost.

In order to gain a deeper insight into the quoted logarithmic dynamical behaviors, let us introduce and discuss a simple model which describes the evolution of a system of particles which hop on a lattice of $n = 0, \dots, N$ stacked planes according to the ideas of parking introduced in [10,12]. We consider a system of particles which can move up or down between N layers in such a way that their total number is conserved. We ignore the correlations among particles rearrangements and the problem related to the mechanical stability of the system. The master equation for the density on a generic plane n , except for the $n = 0$ plane, is given by

$$\begin{aligned} \partial_t \rho_n = & (1 - \rho_n)D(\rho_n)[\rho_{n-1}p_{\text{up}} + \rho_{n+1}p_{\text{down}}] \\ & - \rho_n[(1 - \rho_{n-1})D(\rho_{n-1})p_{\text{down}} \\ & + (1 - \rho_{n+1})D(\rho_{n+1})p_{\text{up}}], \end{aligned} \quad (3)$$

where p_{down} and p_{up} have been defined above for the Tetris-like model. $D(\rho_n)$ is a sort of mobility for the particles given by the probability that the particle could find enough space to move. Apart from other effects it takes mainly into account the geometrical effects of frustration, i.e., the fact that the packing prevents the free move of the particles. In a naive way one could imagine a functional form like $D(\rho_n) = \rho_n(1 - \rho_n)$ obtained by considering only the nearest neighbors interactions in the Tetris-like model. It is easy to realize that such an approach does not account for the complexity of the problem where the packing at high densities creates long range correlations in the system, and, using this functional form, the equations show a trivial exponential relaxation. Nontrivial results are obtained with a careful choice of the functional form for $D(\rho_n)$ which takes onto account the cooperative effects on the dynamics generated by the frustration. This functional form can be obtained by evaluating the rate specifying how many steps are needed in a frustrated system, i.e., the Tetris-like model, with respect to a nonfrustrated one, to achieve a rearrangement in a new configuration. We do not report here the

complete calculation of this rate which involves the evaluation of the configurational entropy of the frustrated and of the nonfrustrated systems, respectively, and we refer to [17]. It is, nevertheless, particularly enlightening to consider the example $N = 2$. In this case the system can be reduced to a one-dimensional chain in which the average length of the filled intervals turns out to be given by $\langle l \rangle \simeq \rho/(1 - \rho)$. The number of steps to move a certain particle, related to the number of steps necessary to move the entire interval (of average length $\langle l \rangle$) aside that particle, will be the order of $N_\rho \sim \exp(l)$. The general form of $D(\rho_n)$, although very complicated, must then include a term like

$$D(\rho_n) = D_0 \exp[-\rho_n/(1 - \rho_n)]. \quad (4)$$

We checked this functional form, which can be seen how the outcome of a free-volume theory for granular media [10,11,17], by means of specific simulations for that quantity on the Tetris-like model [15].

In the general case with arbitrary N we obtained the exact asymptotic stationary solution for the density on each plane. This solution is in an implicit form and for that we refer to [15]. It is possible, nevertheless, to extract the approximate explicit behaviors. In particular, if M is the total “mass” of the system, i.e., the maximal number of planes which can be completely filled, one gets

$$\begin{cases} \rho_k^\infty \simeq 1 - 1/[(M - k) \ln(1/x)] & \text{for } k \ll M, \\ \rho_k^\infty \simeq e^{(M-k) \ln(1/x)} & \text{for } k \gg M. \end{cases} \quad (5)$$

The stationary solution tends thus to a step function $\theta(k - M)$ in the limit $x \rightarrow 0$.

Let us now comment on the dynamical behavior of the system, i.e., the relaxation towards the stationary solution. We start by considering the simplest case with just $N = 2$ planes. In the limit $x \equiv p_{\text{up}}/p_{\text{down}} \ll 1$ and for a sufficiently high total density $\rho = 1 - \epsilon$ ($\epsilon \ll 1$), one can easily prove [15] that the asymptotic equilibrium lower plane density behaves like $\rho_1^\infty \simeq 1 + 1/\ln[xf(\epsilon)]$, where $f(\epsilon) = 2\epsilon/(1 - 2\epsilon) \exp[-(1 - 2\epsilon)/2\epsilon]$. The dynamical equation for ρ_1 can be written exactly. In the limit $\rho_1 \gg (1 - 2\epsilon)$ (which holds for sufficiently long times) this equation exhibits a very simple form as

$$\partial_t \rho_1 = B(x, \epsilon)(1 - \rho_1)D(\rho_1) - A(x, \epsilon)\rho_1, \quad (6)$$

with $B(x, \epsilon) = (1 - 2\epsilon)/(1 + x)$ and $A(x, \epsilon) = 2\epsilon \exp[-(1 - 2\epsilon)/2\epsilon]x/(1 + x)$. This equation has the same form of the one-dimensional “parking problem” studied in [10] whose absorption and desorption parameters are now written in terms of the global density of the system $1 - \epsilon$, and of the vibration amplitude ratio x . It exhibits a logarithmic solution up to times of the order of $t_0 \sim 1/A(x, \epsilon)$ [10]. Later on, when the density approaches its steady state value, the first term on the right-hand side of Eq. (6) becomes negligible with respect to the loss term, and an exponential saturation becomes dominant. Here we just note that t_0 grows inversely proportional to x but has an essential singularity for ϵ

going to zero. So for low enough amplitude vibrations or high enough densities the logarithmic region extends actually up to any experimentally observable time. The cooperative effect of interaction among the different planes makes the times over which one observes the logarithmic relaxation longer and longer. Crucial for this effect is the value of ϵ , i.e., the asymptotic difference of density between two adjacent planes. In the general case of N planes, one has from Eq. (5) that in the bulk, for finite values of x , $\epsilon_k \approx x^{M-k}$, i.e., the ϵ_k are exponentially small in M . We then expect that the logarithmic relaxations extend up to times of the order of x^{-M} (see [15] for a detailed discussion of this point).

Let us now notice a further aspect of our model. The two-step dynamics of our model may be easily interpreted in terms of a Glauber dynamics for a Hamiltonian with Ising-like variables. In this language the geometrical model is mapped into the following Ising-like Hamiltonian with vacancies in the limit $J \rightarrow \infty$:

$$H = \sum_{\langle ij \rangle} J[S_i S_j - a_{ij}(S_i + S_j) - 1]n_i n_j + g \sum_i y(i), \quad (7)$$

where $n_i = 0, 1$ are occupancy variables and $S_i = \pm 1$ are spin variables that corresponds to the twofold orientation of the particles. $a_{ij} = \pm 1$ are fixed nonrandom bond fields with ordered structures: $a_{ij} = 1$ for bonds along one direction of the lattice and $a_{ij} = -1$ for bonds in the other. In the gravitational term $-g \sum_i y(i)$, g is the gravity, and $y(i)$ is the ordinate of the lattice site i . It is easy to realize that the sum of the a_{ij} converging on each single site is zero. This implies that the ground state of Hamiltonian (7) is perfectly antiferromagnetic if the densities of the two kinds of particles are equal. This state is reached just when all the sites of the lattice are occupied, so $n_i = 1 \forall i$. This mapping, and the ones for the models with a variety of shapes which lead to Potts-like Hamiltonians, are particularly useful as starting points for an analysis of these systems in a thermodynamic framework [15].

In this paper we have introduced a very simple geometrical model in order to describe the phenomenon of compaction in dry granular media. It takes into account excluded volume effects, say the geometrical constraints which are felt by granular media during the relaxation towards the highest density optimal packing configuration. When subjected to Monte Carlo vibrations, defined by a diffusive dynamics, it exhibits a density compaction after tapping which reproduces the inverse logarithmic behavior found in both experiments [5] and other models [8–10].

This Tetris-like model can be easily generalized by introducing an arbitrary fixed number of shapes for the particles which correspond to complicated matrices for the particle-particle interactions. This kind of generalization does not change the qualitative structure of the relaxation,

but it could account for other effects of disorder in granular media: segregation, hysteresis, etc. [15].

Furthermore, we presented a simple dynamical model of N planes exchanging particles with excluded volume effects. For this model we have found the exact stationary density distribution and we have shown how, without loss of generality with respect to the choice of particular geometrical constraints, it allows for an explanation of the inverse logarithmic law for compaction.

It is, moreover, interesting that the pure geometrical model presented here can be mapped into a simple Hamiltonian formalism of an Ising antiferromagnet. This connects our work to previous works [3,9,10] introduced to discuss different aspects of granular media phenomenology, and could open the way to their systematic analysis [15].

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