Effects of relaxation processes during deposition of anisotropic grains on a flat substrate

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The ballistic deposition on a one dimensional substrate of grains with one degree of freedom, called spin, is studied with respect to relaxation processes during deposition. The "spin" represents the grain anisotropy, e.g. its longest axis with respect to the vertical. The grains interact through some contact energy ($J$) and are allowed to flip with a probability $q$ during deposition and relaxation. Different relaxation processes are investigated. The pile structure is investigated, i.e. the density and "magnetisation", as a function of $q$ and $J$. A percolation transition is found across which the cluster size changes from exponential-like to a power law-like dependence. The differences between "ferromagnetic" and "anti-ferromagnetic"-like contact energies are emphasized as a function of $q$.

I. INTRODUCTION

The sandpile problem \cite{1} is one of the most recently often tackled problems in the self-organisation of complex systems. There are several questions of interest, not only concerning the density, compaction, stability, intrinsic dynamics, etc. but also concerning the detailed non equilibrium physics inherent to such systems \cite{2}. Experimental observations pertain to the force structure \cite{3} in the pile and to the clustering or percolation properties of grain piles \cite{4}. It is known that the system is hyperstatic \cite{5}. In fact the systems are not at all in equilibrium in a thermodynamic sense, resulting in hysteresis and ageing processes. A description of the construction of the pile is thus a relevant input before further studies.

One important physical constraint to be considered in describing granular piles is that the materials are not made of symmetrical (spherical or cubic) entities \cite{6}. Whence grains can be imagined to be identical entities but having one degree of freedom, call it a spin, for usual statistical mechanics considerations. Such a "spin" allows us for referring to a direction or a rotation process. The spin indicates, e.g. the orientation of the longest grain axis with respect to the vertical.

We have studied such a model \cite{7,8}, within a (magnetic) ballistic deposition process; it is similar to the Tetris model \cite{9}, but more simplified. Basically the (2-dimensional) grains are anisotropic and are deposited vertically as in a gravity controlled rain. For simulation studies we have imagined a two dimensional vertical silo like a triangular lattice with vertical edges, but with periodic boundary conditions. The grains can be submitted to an external field during deposition such that their orientation can change (or not) at each step, with a certain probability. The grain energy is calculated at each falling down step according to a sort of Ising energy, the exchange integral being a map of the contact energy between grains. The latter can have various origins: surface roughness, local charges, mechanical, chemical, dipolar or magnetic effects, ... . It is known that (long range) magnetic interactions lead to clustering and aggregation \cite{10}. For simulation ease, we can limit the interactions to a short range.

We have previously examined clustering effects as in \cite{11,12}, through the cluster fractal dimension, the pile overall density, the distribution of grain orientations, ... and have found through percolation arguments \cite{13} the existence of different cluster growth "mechanisms".

However, except for a Metropolis like dynamical condition \cite{14} during the Monte Carlo simulation, we have not fully let the system relax during the deposition. This constraint is hereby removed. We have performed simulations under two pile relaxation conditions to be described in Sect. II. One is a total gravitationally controlled relaxation, the other is a blocked gravitationally controlled relaxation, relaxing the ballistic constraint, and allowing for the grain to move to a neighboring column. It should be expected that such a relaxation has a coarsening effect.

The results are found in Sect. III while Sect. IV contains some brief conclusion.

II. EXPERIMENTAL PROCEDURE

A few changes to the experimental procedure presented in \cite{6} are hereby introduced. We propose an algorithm for creating a pile with a fixed probability $q \in [0;1]$ for spin flip. The algorithm for arbitrary $q$ (so called $q$-MBD model, in contrast to the $1/2$-MBD model \cite{6}) goes as follows:

1. first, we choose a 1-dimensional crenellated horizontal substrate of spins with a predetermined (hereby random) configuration; periodic boundary conditions are used; on each site a vertical column of empty cells is placed. The lattice symmetry is thus hexagonal.

2. a falling (up or down) spin is dropped along one of the lattice columns from a height $r_{\text{max}} + 5a$, where $r_{\text{max}}$ is the largest distance between an occupied
cluster site and the substrate, i.e. the height of the highest column growing from the substrate on the lattice.

3. more importantly at each step down the spin can flip i.e., change its "sign", with probability $q$: more specifically the probability to choose the "up" direction is $q$.

4. the spin goes down flipping until it reaches a site perimeter of the cluster at which time the local gain in the Ising energy (in absence of an external field)

$$\beta E = -\beta J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

(1)

thus for possible cluster growth is calculated. The exchange integral $J$ describing spin-spin interaction can be thought in granular matter to be like some contact energy due to the surface roughness or the elastic, electric, magnetic, chemical ... character of grains; it can be also a measure of some mis-orientation entropy. If the energy gain is negative the spin sticks to the cluster immediately (sticking probability =1.0) and one goes back to step 2. In the opposite case the spin sticks to the cluster with a rate $\exp(-\Delta \beta E)$ where $\Delta \beta E$ is the local gain in the Ising energy. If the spin does not stick to the cluster it continues going down under the same stick and fall rules. At some step the spin sticks to the cluster. If the site just below the falling spin is occupied the spin is allowed to relax by moving down in one of the nearest columns.

5. At this point we introduce and study three kinds of relaxation processes:

   I. No relaxation – the no-relaxation process is the pure $q$-MBD, i.e. the spin sticks to the cluster immediately.

   II. Total gravitationally controlled relaxation – in the total gravitational relaxation process, when the spin reaches the cluster, i.e. the site just below the spin is occupied, the spin can, with equal probability: stay on the site, or roll down all the way in the left or the right neighbouring column if one of the first neighboring sites is unoccupied. The spin continues rolling down until it reaches a site from which the rolling is not possible; one assumes that the rolling process is due to the gravity without any resistance.

   III. Blocked gravitationally controlled relaxation – after reaching the cluster the spin can, with equal probability: stay on the site, roll down on the left or on the right from the site as for the total gravitational relaxation (II), but can also stick to the pile on its way to the lowest level: During every move towards the lowest level the falling spin can be stopped and stick to the cluster depending on the local gain in the Ising energy.

6. After the spin sticks to the cluster one goes back to step 2.

After dropping a (large) number of spins the physical quantities of interest like magnetization, density, histogram of up/down spin cluster size, histogram of hole cluster size, etc. are computed.

III. NUMERICAL RESULTS

All results reported below are for a triangular lattice with vertical edges of horizontal size $L = 100$, i.e. the width of the seed substrate, and when the pile made of clusters has reached a 100 lattice unit height. The substrate consists of spins with either direction chosen with probability $q$. Every reported data point hereby corresponds to an average over 1000 simulations.

A. Density

We define the density of a cluster as

$$\rho = \frac{\text{number of spins in the cluster}}{\text{number of sites on the lattice}}$$

in which obviously the number of lattice sites in the denominator = 10000.

Figs. 4 illustrate the behaviour of the density with respect to the $q$ and $\beta J$ parameters. The figures convince us that the density reached by the pile in the presence of relaxation is always higher than in absence of relaxation, at fixed $q$ and $\beta J$ values, as expected. The reached density values are not trivial though (compare with 13). It can be noticed, as expected also that $\rho^{II} > \rho^{III} > \rho^I$ whatever the interaction sign.

B. Magnetization

The dependence of the magnetization defined as

$$M = \frac{n_+ - n_-}{n_+ + n_-}$$

(2)

is shown in Fig. 5(a) as a function of $\beta J$ and $q$, where $n_+$ and $n_-$ are the number of up and down spins respectively, i.e. $n_+ = 10000\rho_+$. This quantity can be considered as a measure of the difference in grain orientations in the packing, when the spin (+) is understood
FIG. 1: Projections of the total spin (or grain) density dependence on $q$ and $\beta J$ where $\beta J > 0$: (a) case I, (b) case II, (c) case III.

FIG. 2: Projections of the total spin (or grain) density dependence on $q$ and $\beta J$ where $\beta J > 0$: (a) case I, (b) case II, (c) case III.

e.g. as indicating that the grain longest axis orientation is along the vertical.

In [6] a non-linear-like dependence on $q$ was found for the magnetization though with small departure from linearity due to the changes in the interaction strength. Notice that the relaxation processes make the departures from linearity still smaller; the smallest departures exist in the case II, total gravitational relaxation (Fig. 3b). As it was mentioned in [6] this has to be expected if one recalls that $q$, in a first approximation, is the fraction of deposited up-spins.

C. Percolation

In this section we present results concerning the percolating cluster (from the substrate to the top of the pile) of a typical entity, i.e. the up-spins. In order to do so every pile built by the algorithm has been checked in order to determine whether there is a percolating cluster of up-spins. At fixed $q$ and $\beta J$ the fraction of piles consisting of this given type of percolating cluster was computed. This value is thought to be representative of the critical percolation $p_c$.

Fig 4 shows the behaviour of $p_c$ with respect to $q$ for several values of the $\beta J$ parameter for the three cases. The sigmoid curve is likely due to the finite size of the system. Observe that the interval of $q$ for which $0 < p_c < 1$ is wider when relaxation occurs. One can also observe that the cases AF or F and $\beta J = 0$ are much more distinguishable when there is relaxation (total or blocked gravity). However some convergence toward some finite $p_c$ value seems to occur for increasing $|\beta J|$, as seen on Fig. 5 for case II, – the asymptotic value depending in each case on $\beta J$ sign and being at a lower $q$ value when $\beta J > 0$.

Notice that for $\beta J > 0$ in the relaxation cases percolation occurs for $q > 0.59 = q_0$ (Fig 4b) while in the non-relaxation case it exists for $q > 0.8 = q_0$ (Fig 4a). Therefore, relaxation has an obvious essential influence on the critical percolation value. Recall that in a first approximation the $q$ parameter is the percentage of up-spins in the pile, therefore a lower value of $q_0$ means that one does not have to use a lot of up-spins to have a percolation path (this is useful for example if the up-spin material is much more expensive or dangerous).

D. The size (mass) distribution of clusters

Many problems in granular matter concern the creation of clusters according to segregation[14], creation of avalanches[15] or decompaction[16]. In this section we present the results of the analysis of the size (mass) of spin and hole clusters in this $q$-MBD model with or without relaxation processes.

In [6] it has been found that the number ($N_s$) of clusters dependence on the size ($s$) of the clusters demonstrates a crossover effect, i.e. from an exponential-like to a power law-like dependence. The power law-like regime exists for high $q$ values and the exponential law regime occurs when the $q$ parameter is low. It was conjectured
FIG. 3: The magnetization for (a) the relaxation case I, (b) the relaxation case II, (c) the relaxation case III. Three values of $\beta J$ are presented.

FIG. 4: Dependence of the percolation probability $p_c$ on $q$: (a) the relaxation case I, (b) the relaxation case II, (c) the relaxation case III. Three values of $\beta J$ are presented.

FIG. 5: Dependence of the percolation probability $p_c$ on $q$ for the relaxation case II (total gravitationally controlled relaxation) for: (a) $\beta J > 0$ and (b) $\beta J < 0$.

FIG. 6: The exponent $k_p$ form power law regime: (a) the relaxation case I, (b) the relaxation case II, (c) the relaxation case III.
that the border value is at the critical percolation ($q_c$).

A crossover effect likewise occurs in presence of relaxation. The whole data analysis is not reproduced here; it was done as for the case I in [1]. The differences are particularly noticeable in the power law region i.e. for high values of $q$. Fig 6 shows the behaviour of the power law exponent $k_p$, where $N_s \propto e^{-k_p s}$ and $N_s$ is a number of clusters with mass $s$ for the three models. Notice that the $k_p$ parameter is quasi the same (taking into consideration error bars) for finite $\beta J$ and $\beta J = 0$, when $q > 0.8$, i.e. when $p_c \approx 1$. In that case $k_p$ is almost $q$ independent.

Let us introduce (like in [2]) two parameters to characterize the exponential law regime: an exponent $k_E$ where $N(s) \sim \exp(-k_E s)$ and $A_E$ where $k_E = \exp(-A_E q)$. Observe (Fig 7) in contradistinction with the no relaxation models that $A_E \neq \text{const}$ for $\beta J < 0$, but $A_E \equiv \text{const}$ for $\beta J < -2$. In other words $A_E \equiv \text{const}$ for $|\beta J| < 2$ in the presence of relaxation, i.e. for small values of $q$ the cluster growth does not much depend on the interaction strength for higher interaction vaules.

E. The analysis of spin configurations

The probability of spin sticking for a given spin neighbourhood configuration has been counted. The results reveal that the most probable configurations depend on $q$ and $\beta J$. We have investigated many configurations in the $(q, \beta J)$ plane. We confirm that this approach allows to estimate as well the percolation transition, but such results cannot be fully displayed here.

The probabilities seem to have a very small dependence on the $\beta J$ parameter. However the $q$ parameter induces a strong influence on the configuration probability occurrence. No simple empirical fit has been found for such dependences. For the sake of conciseness and argument we only display two tables (Table II and III) for $\beta J = -5$ and for $\beta J = 5$ respectively for case II and various $q$ values.

We notice that the same configurations are most probable, in both relaxed and non-relaxed cases. The probability of occurrence for the most frequent configuration when $\beta J < 0$ is slightly smaller for the non-relaxed case, but this implies that the other configurations have a higher probabilities and occur more often when there is no relaxation. This entails a larger diversity of possible configurations in absence of relaxation processes. For $\beta J > 0$ the probability of occurrence for the most frequent configuration in the non-relaxed case is not necessarily smaller compared to the II and III case; the differences are slender and may be sensitive to numerical details.

IV. CONCLUSIONS

Granular pile spreading processes are driven by cooperative non-linear evolution rules. This leads to develop patterns which often reach a high level of complexity. We have combined topology and mass (or size) in order to describe granular piling in a simple way on a 1-D substrate. The grains are taken to be anisotropic, and the pile forming through a ballistic deposition process at first. However, in order to take into considerations and observations by wonderful colleagues from the pharmacy department [17], we have allowed the granular pile to somewhat relax, in removing the constraint of ballistic deposition when the grain reaches the pile. We have allowed for its downward motion along neighbourhood columns.

The pile density of course increases with relaxation. The size distribution of clusters follows intricate laws. Above a percolation transition, a power law distribution is found, but it is like an exponential law below. Such a transition occurs at non trivial values in the $(q, \beta J)$ plane. Slight cluster configuration differences exist whether the "spin-spin interaction energy" is positive or negative.

The above changes in density could be usefully cross-checked with new experimental studies. This would give some information on the constact energy $\beta J$ and the spin-spin probability, the latter through the measurement on the falling spin. Time dependent effects should now be usefully investigated both in simulations and in experimentally realistic cases. For example Majumdar and Dean [18] found that the magnetization relaxes extremely slowly, in an inverse logarithmic fashion for 1-D chains. The higher dimensionality cases should be of interest. The role of avalanches, as in real sand/grain piling should also be of interest next, even taking into account the toppling of clusters of granules [19].

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[1] P. Bak, How Nature Works: the Science of Self-organized Criticality (Springer, Berlin and New York, 1996).
[2] H. J. Herrmann, in Physics of dry granular media, edited by H. J. Herrmann, J.-P. Hovi, and S. Luding (Kluwer, Dordrecht, 1998).
[3] J. H. Snoeijer, M. van Hecke, E. Somfai, and W. van Saarloos, Phys. Rev. E 67, 030302 (2003).
[4] A. Vazquez and O. Sotolongo-Costa, Phys. Rev. E 61, 944 (2000).
[5] A. Mehta and J. M. Luck, J. Phys. A 36, 365 (2003).
FIG. 7: The exponent $A_E$ form exponential law regime: (a) the relaxation case I, (b) the relaxation case II, (c) the relaxation case III.

TABLE I: The distribution of typical configurations in the case (II) for $\beta J = 5$; conf. type corresponds to a configuration type (see Fig.5); prob. corresponds to a probability magnitude for the configuration type. The symmetrical (with respect to vertical axis) configurations are not recognized, i.e. 0-000 and 000-0 are the same configuration types.

| q=0  | q=0.25 | q=0.5  | q=0.75 | q=1.0  |
|------|--------|--------|--------|--------|
| conf. type | prob. | conf. type | prob. | conf. type | prob. | conf. type | prob. | conf. type | prob. |
| 000+0 | 0.917  | 000+0  | 0.694  | 000+0  | 0.340  | 000-0  | 0.694  | 000-0  | 0.917  |
| 0+0+0 | 0.165  | 0+0+0  | 0.102  | 0+0+0  | 0.339  | 0-0-0  | 0.102  | 0-0-0  | 0.166  |
| -0-++ | 0.000  | 000-0  | 0.060  | 0-0-0  | 0.068  | 000++  | 0.018  | 000++  | 0.000  |
| -0-+0 | 0.000  | 000++  | 0.046  | 000++  | 0.036  | 000-0  | 0.036  | 000-0  | 0.036  |
| -0+++ | 0.000  | 0-0-0  | 0.039  | 0-0-0  | 0.036  | 0-0-0  | 0.039  | 0-0-0  | 0.039  |
| -0--+ | 0.000  | 000-0  | 0.035  | 0-0-0  | 0.035  | 000--  | 0.035  | 000--  | 0.035  |
| -0-0+ | 0.000  | 000++  | 0.027  | 0-0-0  | 0.035  | 000--  | 0.027  | 0-0-0  | 0.027  |
| -0-0- | 0.000  | 000+0  | 0.009  | 000+0  | 0.035  | 000--  | 0.035  | 000--  | 0.035  |
| 0000  | 0.000  | 0000+  | 0.005  | 0000+  | 0.035  | 000+0  | 0.006  | 000+0  | 0.006  |
| -00++ | 0.000  | 0++00  | 0.005  | 0++00  | 0.018  | 0-0-0  | 0.005  | 0-0-0  | 0.005  |

[6] K. Trojan and M. Ausloos, Physica A 326, 491 (2003).
[7] K. Trojan, M. Ausloos, and R. Cloots, Int. J. Mod. Phys. C 15, 1121 (2004).
[8] E. Caglioti, V. Loreto, H. J. Herrmann, and M. Nicodemi, Phys. Rev. Lett. 79, 1575 (1997).
[9] R. Pastor-Satorras and J. M. Rubi, Phys. Rev. E 51, 5994 (1995).
[10] D. Stauffer and A. Aharony, Introduction to Percolation Theory (Taylor and Francis, London, 1994).
[11] G. Kordrat and A. Pekalski, Phys. Rev. E 65, 051108 (2001).
[12] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).
[13] J. Faraudo, Phys. Rev. Lett. 89, 276104 (2002).
[14] Y. Grasselli and H. J. Herrmann, Granular Matter 1, 1121 (2004).
[15] A. L. Stella and M. D. Menech, Physica A 295, 101 (2001).
[16] G. Oron and H. J. Herrmann, Phys. Rev. E 58, 2079 (1998).
[17] L. Delattre and C. Bodson, private communication.
[18] S. N. Majumdar and D. S. Dean, Phys. Rev. E 66, 056114 (2002).
[19] D. A. Head and G. J. Rodgers, J. Phys. A 31, 107 (1998).
TABLE II: The distribution of typical configurations in the case (II) for $\beta J = -5$; conf. type corresponds to a configuration type (see Fig.8); prob. corresponds to a probability magnitude for the configuration type. The symmetrical (with respect to vertical axis) configurations are not recognized, i.e. 0-000 and 000-0 are the same configuration types.

| q=0 | q=0.25 | q=0.5 | q=0.75 | q=1.0 |
|-----|--------|-------|--------|-------|
| conf. type | prob. | conf. type | prob. | conf. type | prob. | conf. type | prob. | conf. type | prob. |
| 000-0 | 0.986 | 000+0 | 0.356 | 000+0 | 0.340 | 000-0 | 0.355 | 000+0 | 0.989 |
| 000-0 | 0.011 | 000-0 | 0.312 | 000-0 | 0.339 | 000+0 | 0.313 | 000+0 | 0.009 |
| 000-- | 0.003 | 0-0+0 | 0.070 | 0-0+0 | 0.068 | 0-0+0 | 0.069 | 000++ | 0.002 |
| 0-0-0 | 0.002 | 000+- | 0.062 | 000+- | 0.036 | 000+- | 0.063 | 0+0+0 | 0.001 |
| -0++ | 0.000 | 0-0-0 | 0.049 | 000-- | 0.036 | 0+0+0 | 0.048 | -0++ | 0.000 |
| -0-- | 0.000 | 000-- | 0.042 | 000+0 | 0.035 | 000++ | 0.043 | -0-- | 0.000 |
| -0--- | 0.000 | 0000+ | 0.021 | 0000+ | 0.035 | 0000+ | 0.036 | -0--- | 0.000 |
| -0-0+ | 0.000 | 0000+ | 0.020 | 000-0 | 0.035 | 0-0-0 | 0.020 | -0-0+ | 0.000 |
| -0-0- | 0.000 | 000+- | 0.016 | 000++ | 0.018 | 000-- | 0.016 | -0-0- | 0.000 |

FIG. 8: The label notations for Tables II and III, the arrows denote a spin sign (+ is up), if on the site there is any spin; an empty site is "0", the black circle denotes the sticking spin. On the right for both pictures the corresponding configuration type is written.