Statistical models for granular materials

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Abstract

Granular materials, like sand or powders, have many peculiar properties, most of them not yet fully understood. These are due to the special physical properties of granular media like dissipation, friction, dilatancy and the possibilities of having grains of many different sizes and shapes. In the last 10 years much progress has been achieved in the basic understanding of granular media due to the use of tools from Statistical Physics, including disordered systems, critical phenomena, instabilities and chaos. We will present in this talk two examples:

Models for compaction which very much resemble those of structural glasses and predict the logarithmic time dependence experimentally measured in Chicago.

Models that describe the evolution of free surfaces giving the angle of repose, invariant shapes with logarithmic tails and stratification patterns in agreement with observations.

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1 Introduction

Granular materials are very common in our daily life but also important for technological applications and in Geophysics. They have been studied until the last century by physicists including Faraday, Maxwell and Reynolds, but then due to the difficulties in formulating a continuum theory for their deformation, been abandoned by physicists for many decades and only rediscovered about ten years ago. In the meantime (i.e. since the fifties) several engineering companies (soil mechanics, chemical engineering) have succeeded in formulating continuum equations of motion that work rather well in the dense [1] and in the dilute limits [2] of granular systems. But the foundation of these theories is in view of modern statistical mechanics still quite open and has in fact recently become a very active research field. Most importantly, these theories are not applicable in most of the realistic situations in which the granular material changes its density spontaneously and in which different types of grains include interesting segregation patterns.

Statistical physicists have discovered granular media through various independent paths. Fascinated by Faraday's experiment of spontaneous heap formations on vibrating plates [3], a community around P.G. de Gennes investigated various instabilities with similarities in fluid mechanics. Inspired by Per Bak's appealing sand pile model for self-organized
criticality [4], avalanching and intermittency have been measured and modeled. Also the
upcoming of very powerful computers allowed for the simulation of the trajectories of
millions of grains making it possible to study collective phenomena in detail.

The contributions of physicists to various aspects of granular materials has been con-
siderable in the last ten years and is bound to increase much more in the future since the
number of open questions and of new effects seems to increase [5], [6], [7]. One example
has been the discussion about the force transfer in granular packings, building on ideas on
arching from Sir Sam Edwards [8], various models were proposed to describe anomalies of
the stress distribution below heaps, opening a discussion on the description of the internal
texture and the opening of contacts (no-tension elasticity). Novel patterns including
solitons (so-called "oscillons") [9] were discovered for surface waves of vibrated beds. The
Brazil nut effect, i.e. the rising of larger particles under vibration was understood at least in
most situations. The spontaneous formation of density waves in pipe flow was related
to traffic instabilities and the ticking hour glass [10] was explained. Many more effects
like stratification, ripple formation, convection under vibration, shear bands and fingering
have also been better understood.

We want to present in this talk only two examples of the application of statistical
models to granular materials: compaction under vibration and the shape of sandpiles.

2 Models for compaction

A packing of grains can be stable in many configurations which can also have different
global densities. One considers that random assemblies of grains can have a density \( \rho \)
between \( \rho_{\text{dp}} \) and \( \rho_{\text{rp}} \) where \( \rho_{\text{dp}} \) is the lowest density packing and \( \rho_{\text{rp}} \) is the random dense
packing. The first is obtained by carefully opening the structures as much as possible
(e.g. with blown air or at micro-gravity) and the second one is obtained by a suitable
shaking procedure. None of the two limiting densities is sharply defined nor known with
experimental high precision. They depend not only on the grain mixture (which can have
different sizes and shapes) but also on the history of preparation and the details of the
experimental device.

Technologically it is of large interest to produce powders as compact as possible. These
are used for instance in high strength ceramics, ultra strong beton or in sintering of
metal powders. So, vibration techniques to compactify granular systems have evolved
to a technological branch of its own called vibratory compacting [11,12] and which was
particularly advanced in the ancient Soviet Union. Procedures and "cooking rules" are
known of how to change frequency, amplitude orientation and shape of a vibration to
improve the density of granular packings [13,14]. Still, however, no systematic physical
understanding of processes behind compaction had been achieved until recently.

An experimental group in Chicago has performed [15] in the last years very careful
experiments on the compaction of glass beads and other powders in vertical columns
submitted to controlled taps and studied systematically a dependency of the density on
the duration, intensity and history of the tap sequence. The density was measured with
high sensitivity by capacitors and data acquisition went over weeks.

They found that the density increased on average in time following a logarithmic law
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given by

\[ \rho(t) = \rho_\infty - \frac{\rho_\infty - \rho_0}{1 - \ln(1 - \frac{t}{\tau})} \]  \hspace{1cm} (1)

where ρ_0 is the initial density, ρ_\infty the final density and τ the characteristic time. They also
observed that the final density depended on the speed of "quenching", i.e. the velocity with
which the amplitude of the taps was increased and later decreased in time. Furthermore,
they observed that only after an amplitude dependent time, a reversible branch in the
inagram density against amplitude can be reached. These discoveries strongly point to
imilarities to structural glasses.

In view of the many degrees of freedom and the disordered nature of granular packings,
it is clearly a formidable task for statistical physicists to determine ground states and the
behavior under vibrations which could be regarded as a (anisotropic) temperature. Simple
models based on the picture of compaction as upmotion of voids have been suggested and
it was shown that if a Poisson distribution of void sizes is assumed, the logarithmic law
of equation (1) can be derived [16]. Another simple model which asymptotically also
gives eq. (1) is based on a one-dimensional parking model with evaporation [17]. This model
can be generalized to many layers (parking lanes) on top of each other, giving also the
density profile as function of height as done by E. Caglioti and collaborators [18].

All these models are of mean field type and unable to describe the effects of dimension-
ality, walls, different types of vibrations or different types of grains. To be able to modelize
experimental data in more detail, new models, inspired originally by models of structural
glasses, have been proposed recently. These models take into account the frustration to
reach full compaction due to the steric hindrance of the grains.

One model similar to the frustrated percolation model introduced by Nicodemi and
collaborators [19,20] assumes a lattice with bonds carrying quenched numbers J_{ij} = ±1
which give rise to the abovementioned frustration. Particles carrying a spin \sigma_i = ±1
move down (direction of gravity) on the lattice as long as they find a free place below them.
The lattice is a square lattice tilted by 45° so as to allow two equivalent ways to go down.
However, there is the constraint on each bond given by product

\[ J_{ij} \sigma_i \sigma_j = 1 \]  \hspace{1cm} (2)

where \sigma_i and \sigma_j are the spins of the particles sitting on the nearest neighbouring sites i
and j. Evidently a particle can not occupy the side on which another particle already sits.
But a particle can also not occupy an empty side if this occupancy would entail one of
the bonds non fulfilling the constraints of equation (2).

The dynamics described up to now only allows for particles to move down. If they fall
on the bottom of a container (wall at lower boundary), they will form a packing which
after some time will not change anymore (be stable). To describe the vibrations of the
system, a Monte Carlo procedure is implemented in the way that particles can also move
upwards with probability x. The value of x (0 < x < 1) is a measure for the strength
(amplitude) of vibration. It was found with this model that the density increased at given
x like equation (1) in time [18]. The parameters τ and ρ are functions of x such that
there is a characteristic x_0 at which ρ steeply changes to a value close to ρ_{dp}. τ decreases
with $x$ like a power law with a power that changes at $x_0$. This is in close agreement with experimental results. This model also allows to determine the density profile as a function of the height which is consistent with a Fermi-Dirac distribution as obtained also with the layered parking model [18] and also from theoretical considerations [21]. The model also describes the dependency of the final density on a quenching velocity and the reversible branch as found experimentally [19]. Therefore it seems that the present model is very adapted to describe compaction although it has some unrealistic properties like the lattice with quenched variables $J_{ij}$ which of course does not exist in nature.

A model which does not have this defect and still reproduces the entire experimental phenomenology is Tetris [18]. In this model which still works on a tilted square lattice, frustration is not induced by quenched variables, but by the degrees of freedom living on each particle. Each particle has certain “legs”, i.e. bonds which it occupies in the sense that no other particle can have its leg on this bond. An example of such a configuration can be seen in Fig. 1. One can have different species of particles defined by different numbers or directions of the legs as seen in Fig. 1 which allows to study particles of different size, shape or orientation.

Tetris gives the same compaction behavior as the frustrated percolation model discussed above, i.e. the dynamics follows eq. (1) and the final density depends on the quenching velocity [18]. Within Tetris one can also study the effects of different grain species during compaction. It was found that typically the particles segregate such that those with more legs accumulate at the top (opposed to gravity) [22]. This effect is similar to the so-called Brazil nut effect in which larger particles rise from the bottom under vibration. The reason seems to be that particles with more legs impose more constraints and therefore are typically surrounded by more voids. Regions containing such particles are then lighter
size of particles. From ref. [22], s is in close agreement with density profile as a function m as obtained also with the atoms [21]. The model also velocity and the reversible t the present model is very x properties like the lattice nature.

The entire experimental s on a tilted square lattice, degrees of freedom living on ich it occupies in the sense e of such a configuration can xed by different numbers y particles of different size, percolation model discussed r depends on the quenching different grain species during a such that those with more ct is similar to the so-called tton under vibration. The r constraints and therefore ch particles are then lighter

Fig. 2. Size distribution of internal avalanches using Tetris in double-logarithmic scale, upper curve dimers, lower curve T-shaped particles.

and rise due to buoyancy.

Tetris can also be cast in a Hamiltonian formalism with Potts variables describing the different species and specific interactions between them which for diverging coupling constants describe the exclusive volume constraints [18]. The model can also be solved in a mean field approximation.

An interesting property of granular packings are internal avalanches and their statistics. They can be generated by removing one grain inside or at the bottom of the packing and watching how many grains consequently move. A modelization of this effect by falling squares gave a power-law in the distribution of avalanche sizes [23] showing the appearance of self-organized criticality [4]. Recently internal avalanches were studied with Tetris [24] by removing single grains at the bottom and putting them back on top. The size distribution again followed a power-law with exponent τ. Interesting is, however, that τ is different if the grains occupy two opposite legs (dimers) or if they have three legs (T-shaped). This can be seen in Fig. 2. The difference in universality class seems to be due to the different degeneracies of the densest configurations (ground states) which is two in the case of dimers and infinity for T-shaped particles.

3 A model to calculate the angle of a heap

One of the striking features of granular materials is the existence of a finite slope, given by the angle of repose θ, below which a free surface is stable. If a sandpile is formed by dropping either grain by grain or a small stream of particles from a point source on a flat table, a beautiful cone is formed having the slope tan θ.

There exists to my knowledge no model capable of calculating the angle of repose of a given set of grains from the properties of these grains, as their size, shape, surface
roughness or material properties, like their coefficient of restitution or elastic moduli. Using the main ingredients of grain motion down the heap surface, we want to discuss in the following a simple model to calculate the heap angle $\theta_H$ [25].

Let us consider particles of diameter one jumping down a stair. Particle $i$ is characterized by an energy $e_i$. When it falls down one step of height $\Delta h$ of the stair, its energy becomes

$$e'_i = (e_i + \Delta h)r$$

where $r$ is the restitution coefficient, i.e. a material property which describes the loss of energy at one collision. In reality, however, a surface has many local minima due to the grain shape and which are more pronounced the larger the grain. We describe these local minima by an energy barrier $U$ that a grain needs to get out of it. So, if $e'_i < U$, the particle does not jump but aggregates to the pile by increasing the height of the stair by unitary. If $e'_i \geq U$, the particle can move ahead. The two microscopic parameters characterizing size, shape, surface roughness and material properties of a grain are thus $r$ and $U$.

It is easy to implement this model numerically and it has been studied intensively [25], [26]. For a single species of particles, i.e. all particles having the same value for $r$ and $U$, one observes that the pile asymptotically becomes a perfect triangle with a well defined slope $\gamma = \tan \theta$. Let us in the following consider this case of a single species in more detail.

$\gamma$ is independent on the initial energy $e_i^{(o)}$ of the particles, i.e. the energies with which the grains hit the top, as long as all particles have the same value for $e_i^{(o)}$. If, however, the initial energies $e_i^{(o)}$ are chosen randomly from a distribution of width $W$, the value of $\gamma$ increases with $W$. This numerical observation can be explained by structures forming on the top of the heap. The shape of the top of the heap depends on the value of $e_i^{(o)}$ and for large $e_i^{(o)}$ craters are observed on the top in agreement with experiments [26].

The value of $\gamma$ increases with $r$ and $U$ in a complicated way as seen in Fig. 3. This devil's staircase behavior is due to the fact that we are essentially constructing the pile on a square lattice on which some slopes are easier to implement than others. An experimental heap would not have that problem and therefore in reality the curve should be smooth and monotonous. We must thus see the devil's staircase as an artifact of the model but believe that the general trend of the curves, i.e. for instance the upper or lower envelopes, reproduces qualitatively the experimental observations.

It has been possible to derive the devil's staircase seen in Fig. 3 analytically [25] and in the following we will sketch the argument. Let us consider first the case $0 < \gamma < 1$. The numerical simulation has shown that a given slope $\gamma$ was made of periodic units of length $L$ and height $N$ such that $\gamma = \frac{N}{L}$. Each unit consists of $N$ individual steps of height one and length $l_j$ such that

$$L = \sum_{j=1}^{N} l_j$$

Since the slope does not change with time, we are in a steady state and at a given place of the stair, all particles moving down have the same energy $e_i$. The values of these energies are such that the steps neither shrink nor grow. This implies for the energy $e_j$ of the last
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(3)
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Fig. 3. Numerically measured angle of repose \( \gamma(r, U) \) as a function of \( U(1-r)/r \) for \( r = 0.3 \) (\( \bullet \)),
0.5 (\( \circ \)), 0.7 (\( \ast \)), and \( r = 0.9 \) (\( \circ \)). The lines display the \( \gamma(r, U) \) as calculated from the iteration
of Eqs. (6-9) (see the text for details).

site of step \( j \) that it must fulfill

\begin{equation}
(5)
\end{equation}

The periodicity of the unit implies

\begin{equation}
(6)
\end{equation}

From Eq. (5) we have for \( l_j \) the following limits

\begin{equation}
(7)
\end{equation}

so that

\begin{equation}
(8)
\end{equation}

where the brackets \([.\ldots]\) mean the integer part. In order to calculate \( \gamma \) one must know \( N \) and \( L \) and that is done by solving the system of \( 2N + 2 \) equations of the variables \( N, L, l_j \) and \( e_j, j = 1, \ldots, N \) given by the \( N \) equations of (5) and (8) and the equations (4) and (6). The result perfectly agrees with the numerical result of Fig. 2.

To deal with \( \gamma > 1 \), it is useful to consider first the special case in which the stair is made of equal steps of length one and height \( n \). Then the steady state condition gives

\begin{equation}
(9)
\end{equation}

This yields \( (U + n)r < U \) and therefore

\begin{equation}
(10)
\end{equation}
Finally, one has to deal with the general case but we refer for that to reference [25].

It can be shown that the above model for a single species is equivalent to a specific one-dimensional Ising model with long range interactions in the limit of zero temperature on a chain of length \( L \) and periodic boundary conditions. The Hamiltonian of that Ising model is

\[
\mathcal{H} = \sum_i U s_i + \frac{1}{2} \sum_{i,j} J (|i-j|) \left( s_i + 1 \right) \left( s_i + 1 \right)
\]  

(11)

where \( s_i = \pm 1 \) and the interaction is given by

\[
J(x) = (1 - r^L)x^x
\]  

(12)

If \( N \) is the number of sites with \( s_i = +1 \), then the \( \gamma \) of our model corresponds to the magnetization \( N/L \). The sites with \( s_i = +1 \) correspond to steps of the stair and \( c_i \) to the interaction energy of spin \( s_i \). The ground state of that Ising model has been obtained some time ago analytically by B\'ak and Bruinsma and (of course) they also found a devil’s staircase [27].

The above model can also be described by continuum equations which with the right choice of boundary conditions can reproduce the crater on the top of a pile for large initial energies \( e_i^{(0)} \) [26].

4 Tails of heaps

A pile constructed by pouring granular material on a table, like the ones shown in Fig. 4, clearly shows deviations from the straight slope which is implied by a constant angle of repose. In particular, on the bottom of the pile there is a tail that seems to avoid a discontinuity of the slope with respect to the table. The upper pictures in Fig. 4 are superposed pictures of a growing pile of sugar in a vertical Hove-Shaw cell at different times made by J. J. Alonso [28]. Each grey scale corresponds to the shape of the pile at another stage of its growth. One recognizes a translational invariance of the shape of the tail, i.e. that the left sides of the contours can be superposed just by horizontally shifting them on top of each other.

The lower picture in Fig. 4 shows the case of lead spheres. One recognizes the shape of the tail with much better resolution than in the case of sugar. It is interesting to note the existence of kinks on the surface (marked by arrows in Fig. 4). In the following we will use the observed translational invariance and the kink picture to derive a formula for the shape of the tail [28].

Let us restrict ourselves to two dimensions and describe a pile by a center part of triangular shape given by the angle of repose and an ensemble of layers of equal thickness \( \delta \) parallel to the surface as shown in Fig. 5, all lengths be measured in units of grain diameters. The layers become shorter the farther they are out giving the envelope a monotonous, concave shape. At the end of each layer one has a kink. The position of the kinks therefore describes the surface of the pile that we want to calculate. The closer the kinks are, the smaller is the slope of the surface. Let us define by \( \xi(h) \) the density of kinks at height \( h \), i.e. how many kinks there are per unit length at height \( h \). Let us call \( \tau(h) \)
that to reference [25].
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\( \xi(h) \) the density of kinks
height \( h \). Let us call \( x(h) \)

\[ \frac{dh}{dx} = \frac{\gamma}{1 + \tilde{\delta}\gamma} \]  (13)

where \( \delta = \frac{\delta}{\sin \theta} \) and \( \gamma = \tan \theta \).

Let \( J(h) \) be the flux of grains at height \( h \). It is largest on the top of the pile and zero at
the end of the tail. The decrease of \( J(h) \) along the surface is due to the fact that grains
aggregate on the surface which corresponds to the growth of the pile. Typically grains
aggregate at the kinks, a fact already mentioned and clearly visible in fig. 4b. This makes
the kinks move up and the corresponding layer grows. Assuming that every particle has
Fig. 5. Schematic picture of the structure of the heap, which grows layerwise, and where there is a kink on the top of each layer.

the same probability of having been aggregated at a given kink, one can define a constant aggregation rate $r$ and describe the change of flux by

$$\frac{dJ}{dh} = rJ\xi$$  \hspace{1cm} (14)

The observed translational invariance implies that during growth the surface moves horizontally at all heights $h$ by the same amount. Since the velocity of the surface, i.e. the rate of aggregation of grains is proportional to the reduction of the flux $J$, one has

$$\frac{dJ}{dh} = B$$  \hspace{1cm} (15)

where $b$ is a constant. Integrating Eq. (15) and considering the boundary condition $J(0) = 0$ gives $J = Bh$. Inserting this in Eq. (14), one obtains $\xi = (rh)^{-1}$, and inserting this in Eq. (13) gives the differential equation

$$\frac{dx}{dh} = \frac{1}{\gamma} + \frac{l}{h}$$  \hspace{1cm} (16)

where $l = \delta/r$. If $h_m$ is the height of the apex of the pile, the boundary condition is $x(h_m) = 0$ and the solution of Eq. (16) is

$$x = \frac{h_m - h}{\tan \theta} + l \ln \frac{h_m}{h}$$  \hspace{1cm} (17)

The first term on the right hand side of Eq. (17) just represents the straight line given by the angle of repose $\theta$. The second term represents the tail on top of that straight part and is due to the kinks. This logarithmic tail extends to infinity but once it is thinner than one grain diameter it cannot be expected to be found in an experiment. So, for practical purposes it has to be cut off at that point.
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\begin{equation}
2 \theta
\end{equation}

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\begin{equation}
\frac{\mu \Gamma}{2h^2}
\end{equation}

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Fig. 6. The deviation of the profile of a polenta heap (markers) from the straight line. The solid line shows the fit to the latter term of Eq. (17), which gives the logarithmic correction to the pile.

The predicted shape of Eq. (17) has been checked experimentally [28]. Since the angle of repose \( \theta \) is known rather precisely, the only fit parameter is \( l \). Such fits are shown as full lines in the upper picture of Fig. 4. A more systematic comparison between the theoretical prediction and the experiment is shown for the case of polenta heaps in Fig. 6. The straight line given by \( \theta \) has been subtracted from the surface so that only the second term of Eq. (17), called \( \Delta x \), is shown in Fig. 6. The agreement is very good. A surprising finding is that for all granular media investigated up to now the fit parameter \( l \) is close to 3. This corresponds to saying that on average one third of the grains aggregates at a kink having the height \( \delta \) of one grain diameter. We have no physical explanation for that number.

Similar logarithmic tails are also found in other geometries like at the outer wall from a silo filled at the center and they are also in agreement with experimental results [29].

5 Conclusion

We have described simple modelizations of grain motion, on one hand in a vibrated packing and on the other hand down on the surface of a heap. In both cases we obtained models that could be mapped to Ising-like Hamiltonians directly showing the connection to classical statistical physics.

Evidently there are still many unsolved problems in granular materials and these are of statistical nature. So it is to be expected that in the future their study will become an important task of statistical physics.
References