Shaken, not stirred: why gravel packs better than bricks

Anita Mehta\textsuperscript{a\textdagger} and J.M. Luck\textsuperscript{b\textdagger}

\textsuperscript{a}S.N. Bose National Centre for Basic Sciences, Block JD, Sector 3, Salt Lake, Calcutta 700098, India

\textsuperscript{b}Service de Physique Théorique, URA 2306 of CNRS, CEA Saclay, 91191 Gif-sur-Yvette cedex, France

We explore the effect of shape – jagged vs. regular – in the jamming limit of very gently shaken packings. Our measure of shape $\epsilon$ is the void space occupied by a disordered grain; we show that depending on its number-theoretic nature, two generic behaviours are obtained. Thus, regularly shaped grains (rational $\epsilon$) have ground states of perfect packing, which are irretrievably lost under zero-temperature shaking; the reverse is the case for jagged grains (irrational $\epsilon$), where the ground state is only optimally packed, but entirely retrievable. At low temperatures, we find intermittency at the surface, which has recently been seen experimentally.

1. Introduction

Why does shaken gravel pack better than shaken bricks do? We explore this question via a one-dimensional model \cite{1,2}; despite its simplicity, it exhibits frustration and slow dynamics, features \cite{3} which link the fields of granular compaction \cite{4,5} and glasses \cite{6}. The central issue that we probe is the effect of granular shape; our main finding is that irregular/jagged and regular/smooth grain shapes have rather different consequences for compaction in the jamming limit.

That glasses or granular media do not have crystalline ground states is well known, as is the fact that their attempts to reach their ground states are ‘jammed’, i.e., hindered by long-range interactions. Our model is based on the following picture of jamming. In the absence of holes (grain-sized voids), the only way that granular media can compact is by grain reorientation. A disordered grain, in our model, ‘wastes space’; that is, it occupies a net volume equal to its size, plus that of a partial void \cite{1,2,7}.\textsuperscript{1} A reorientation of this to an ordered (‘space-saving’) state ‘frees up’ the partial void, for use by other grains to reorient themselves. This cascade-like picture of compaction has been seen in the comparisons with experiment \cite{8} of random graph models \cite{9} of granular compaction. Also, as there \cite{9}, the response of grains to external dynamics is the local minimisation

\textsuperscript{a}anita@bose.res.in

\textsuperscript{b}luck@spht.saclay.cea.fr

\textsuperscript{1}Specifically, in our model, each ordered grain occupies one unit of space, and each disordered grain occupies $1 + \epsilon$ units of space, where $\epsilon$ is a measure of the trapped void space for a given granular shape.
of void space; the ground states so obtained resemble much more the random close-packed state found in granular systems than the rather unrealistic crystalline ground state obtained in earlier work.

2. The model: definition and ground states

Grains are indexed by their depth $n$, measured from the surface of the column. Each grain can be in one of two orientational states – ordered (+) or disordered (−) – the ‘spin’ variables $\{\sigma_n = \pm 1\}$ thus uniquely defining a configuration. We posit an ordering field $h_n$ which constrains the temporal evolution of spin $\sigma_n$, such that the excess void space is minimised – a constraint which is reasonable in the jamming limit.

The stochastic dynamics in the presence of a vibration intensity $\Gamma$ is defined by the transition probabilities:

$$w(\sigma_n = \pm \rightarrow \sigma_n = \mp) = \exp\left(\frac{-n}{\xi_{\text{dyn}}} \mp h_n/\Gamma\right).$$

The dynamical length (or boundary layer) $\xi_{\text{dyn}}$ is a measure of the extent to which free surface effects percolate into the bulk; well beyond this, the dynamics is slow, while within it, the free surface still has an effect on the dynamics which are relatively fast. The local ordering field $h_n$ reads

$$h_n = \varepsilon m_n^- - m_n^+,$$

where $m_n^+$ and $m_n^-$ are respectively the numbers of + and − grains above grain $n$. Equation (2) shows that a transition from an ordered to a disordered state for grain $n$ is hindered by the number of voids that are already above it: in fact $h_n$ is a measure of the excess void space in the system.

In the $\Gamma \to 0$ limit of zero-temperature dynamics, the probabilistic rules become deterministic:

$$\sigma_n = \text{sign } h_n,$$

provided $h_n \neq 0$ (see below). Ground states are the static configurations obeying everywhere. A rich ground-state structure is achieved for $\varepsilon > 0$, because of frustration, whose nature depends on whether $\varepsilon$ is rational or irrational. We mention for completeness that the case $\varepsilon < 0$ is a generalisation of earlier work, with a complete absence of frustration and a single ground state of ordered grains.

The rotation number $\Omega = \varepsilon/(\varepsilon + 1)$ fixes the proportions of ordered and disordered grains in the ground states: $f_+ = \Omega$, $f_- = 1 - \Omega$. For irrational $\varepsilon$, (2) implies that all the local fields $h_n$ are non-zero. Qualitatively, irrational values of $\varepsilon$ denote shape irregularity; the above then implies that for such jagged grains, the excess void space is never zero, or the packing is never perfect, even in the ground state. It turns out that the ground state is in fact quasiperiodic; the local fields $h_n$ lie in a bounded interval $-1 \leq h_n \leq \varepsilon$.

For rational $\varepsilon = p/q$, with $p$ and $q$ mutual primes, $\Omega = p/(p + q)$, and some of the $h_n$ can vanish. This means that grain $n$ has a perfectly packed column above it, so that it is free to choose its orientation. It turns out that orientational indeterminacy occurs at
points of perfect packing such that \( n \) is a multiple of the period \( p + q \). Each ground state is thus a random sequence of two patterns of length \( p + q \), each containing \( p \) ordered and \( q \) disordered grains. The model therefore has a zero-temperature configurational entropy or ground-state entropy \( \Sigma = \ln 2/(p + q) \) per grain. Qualitatively, rational values of \( \varepsilon \) imply a regularity or ‘smoothness’ of grain shape; one could imagine that regular grains would align themselves to fit exactly into available voids where possible, in a ground state configuration. This in fact happens, leading to states of perfect packing at various points of the column and the observed degeneracy of ground states.

3. Zero-temperature dynamics: (ir)retrievability of ground states

Zero-temperature dynamics is a theoretical construct; one assumes that, starting with a random array of objects, the limit of zero shaking intensity will cause their ground state of packing to be achieved. This is neither obvious, nor, as we will show, correct in general.

Our analysis shows [1,2] that, under zero-temperature dynamics, jagged grains are able to retrieve their unique ground state, whereas for regular grains, the true ground states are impossible to retrieve. In the latter case, one finds instead a steady state with non-trivial density fluctuations above the ground states, which recall the observed density fluctuations above the random close-packed state [12,13] in real granular materials. This is intuitively understandable; jagged grains in the limit of extreme compaction can only ‘click’ into place in a unique way, while the huge degeneracy of perfectly packed ground states for regular grains makes any particular one impossible to retrieve, using a random shaking dynamics.

We recall the rule for zero-temperature dynamics:

\[
\sigma_n \rightarrow \text{sign} \, h_n, \quad (4)
\]

For irrational \( \varepsilon \) with an initially disordered state, this results in the recovery and ballistic propagation of the quasiperiodic ground state, starting from the free surface to a depth \( L(t) \approx V(\varepsilon) \, t \). The velocity \( V(\varepsilon) = V(1/\varepsilon) \) varies smoothly with \( \varepsilon \), and diverges as \( V(\varepsilon) \sim \varepsilon \) for \( \varepsilon \gg 1 \) [1,2]. The rest of the system remains in its disordered initial state. When \( L(t) \) becomes comparable with \( \xi_{\text{dyn}} \), the effects of the free surface begin to be damped. In particular for \( t \gg \xi_{\text{dyn}}/V(\varepsilon) \) we recover the logarithmic coarsening law \( L(t) \approx \xi_{\text{dyn}} \ln t \), observed in related work [7,9] to model the slow dynamical relaxation of vibrated sand [12].

For rational \( \varepsilon \), things are more complex; the local field \( h_n \) in \( (4) \) may vanish. We choose to update such orientations according to \( \sigma_n \rightarrow \pm 1 \) with probability 1/2, leading to a dynamics which is stochastic even at zero temperature. Here, even the behaviour well within the boundary layer \( \xi_{\text{dyn}} \) contains many intriguing features, while the dynamics for \( n \gg \xi_{\text{dyn}} \) is again logarithmically slow [12]. Focusing on the limit \( \xi_{\text{dyn}} = \infty \), our main result is that zero-temperature dynamics does not drive the system to any of its degenerate

\footnote{For \( \varepsilon = 1/2 \), for example, one can visualise that each disordered grain ‘carries’ a void half its size, so that units of perfect packing must be permutations of the triad + − −, where the two ‘half’ voids from each of the − grains are filled by the + grain. The dynamics, which is stepwise compacting, selects only two of these patterns, + − − and − + −. Evidently this is a one-dimensional interpretation of packing, so that the serial existence of two half voids and a grain should be interpreted as the insertion of a grain into a full void in higher dimensions.}
ground states. The system instead shows a fast relaxation to a non-trivial steady state, independent of initial conditions. In this steady state, the local fields $h_n$ have unbounded fluctuations as a function of depth [12]; since $h_n$ is a measure of excess void space, this in turn implies the existence of density fluctuations in our model of shaken sand.

Fig. 1 shows the variation of these density fluctuations as a function of depth $n$:

$$W_n^2 = \langle h_n^2 \rangle \approx A n^{2/3}, \quad A \approx 0.83.$$  \hspace{1cm} (5)

The fluctuations are approximately Gaussian, with a definite excess at small values: $|h_n| \sim 1 \ll W_n$. Interestingly, this ‘nearly but not quite’ Gaussian behaviour of density fluctuations in shaken granular media has been seen experimentally [8]; the not-quite-Gaussianness was in the experiment interpreted via correlations, which as we will show below, are also present in our model.

Figure 1. Log-log plot of $W_n^2 = \langle h_n^2 \rangle$ against depth $n$, for zero-temperature dynamics with $\varepsilon = 1$. Full line: numerical data. Dashed line: fit to asymptotic behaviour leading to (5) (after [12]).

To reiterate, (5) implies that the known ground states of a system of regularly shaped grains will never be retrieved even in the limit of zero-temperature dynamics. The steady state will, instead, be one of density fluctuations above the ground state. The present model, to our knowledge, thus contains the first derivation\(^3\) of a possible source of density fluctuations.

\(^3\) A simple scaling argument explains the observed roughening exponent $2/3$. Let $h_n$ be the position of a random walker at ‘time’ $n$. The noise in this fictitious random walk originates in the sites $m < n$ where the local field $h_m$ vanishes. It is therefore proportional to $\sum_{m=1}^{n-1} \text{Prob}\{h_m = 0\}$, hence the consistency condition $W_n^2 \sim \sum_{m=1}^{n-1} 1/W_m$, yielding the power law (5).
fluctuations in granular media \[12,13\], which, here, arise quite naturally from the effects of shape. This prediction of complex experimental observations \[8,12\] is all the more startling given its origin from a model of such simplicity.

We turn now to the issue of correlations. If the grain orientations were statistically independent, i.e., uncorrelated, one would have the simple result \( \langle h^2 \rangle_n = n \varepsilon \), while (5) implies that \( \langle h^2 \rangle \) grows much more slowly than \( n \). The orientational displacements of each grain are thus fully anticorrelated. Fig. 2 shows that the orientation correlations \( c_{m,n} = \langle \sigma_m \sigma_n \rangle \) scale as \[12\]

\[
c_{m,n} \approx \delta_{m,n} - \frac{1}{W_m W_n} F\left(\frac{n-m}{W_m W_n}\right),
\]

where the function \( F \) is such that \( \int_{-\infty}^{+\infty} F(x) \, dx = 1 \). The fluctuations of the orientational displacements are therefore asymptotically totally screened: \( \sum_{n \neq m} c_{m,n} \approx -c_{m,m} = -1 \).

![Figure 2. Scaling plot of the orientation correlation function \( c_{m,n} \) for \( n \neq m \) in the zero-temperature steady state with \( \varepsilon = 1 \), demonstrating the validity of (6) and showing a plot of (minus) the scaling function \( F \) (after [12]).](image-url)

Summing up, we see that the (orientational) displacements of regular grains are anticorrelated\(^4\) within a dynamical cluster \[13\] whose size scales as \( n^{2/3} \). Grains separated by

---

\(^4\)Correspondingly, from a kinetic viewpoint, these results may be interpreted in terms of the time \( n^{2/3} \) spent by a walker bouncing back and forth between the walls of a cage, where his steps are consequently anticorrelated one with the other.
greater than the cluster radius are orientationally screened from each other, i.e., the screening length also goes as $n^{2/3}$. Consistently, the order parameter $Q_n = \langle \sigma_n \text{sign } h_n \rangle$, proportional to the ratio of the screening length to the total length, goes as $n^{2/3}/n \sim n^{-1/3}$.

Similar anticorrelations in grain displacements have been observed in hard-sphere simulations of shaken powders close to jamming \cite{13}; the observation was that grain displacements along the direction of vibration were strongly anticorrelated, while transverse to it, they were uncorrelated. In the absence of free voids, compaction in the simulations happened by the phenomenon of bridge collapse; the vibrations coupled to the longitudinal displacements of the grains, allowing upper and lower grains in a bridge to collapse onto each other, thus minimising the trapped void space between them. This led to the observed longitudinal anticorrelations; the low intensities of vibration on a jammed granular bed did not allow for a coupling with transverse granular displacements. Given the close agreement of these earlier results \cite{13} with our present ones, we can in hindsight justify our choice of a columnar model to model granular compaction in the jamming limit.

Finally, we point out that the landscape of visited configurations in the steady state of density fluctuations has a fractal-like structure \cite{1,2}. Fig. 3 shows that, on whichever scale we look, some configurations are clearly visited far more often than others. It turns out that the most visited configurations are the ground states of the system (empty circles). We suggest that this behaviour is generic: i.e., the dynamics of compaction in the jammed state leads to a microscopic sampling of configuration space which is highly non-uniform, so that the ground states are visited most frequently. This might be expected when the system is constrained to compact. However, it should be noted that under continuous shaking, the system cannot rest in a ground state even when one is found; it evolves constantly, and thereby generates the observed density fluctuations. It should also be noted that the entropy reduction $\Delta S \sim n^{1/3}$ resulting from this fine structure is subextensive, and therefore negligible with respect to the free entropy $S_{\text{flat}} = n \ln 2$. Our model thus provides a natural reconciliation between, on the one hand, the intuitive perception that not all configurations can be equally visited during compaction in the jamming limit; and, on the other, the flatness hypothesis of Edwards, which states that for large enough systems, the entropic landscape of visited configurations is flat \cite{15}.

4. Low-temperature dynamics

We now turn to the investigation of the low-temperature dynamics of the model. Our main finding is the observation of intermittency in the position of the boundary, or surface, layer; this has recently been observed in experiments of vibrated granular beds \cite{16}.

For rational $\varepsilon$, the presence of a finite but low shaking intensity does not change much; the zero-temperature dynamics is in any case stochastic, and low-temperature dynamics merely increases the effect of noise. However, for irrational $\varepsilon$, low-temperature dynamics introduces an intermittency in the position of a surface layer, which separates a quasiperio-
Figure 3. Plot of the normalised probabilities $2^{12} p(C)$ of the configurations of a column of 12 grains in the zero-temperature steady state with $\varepsilon = 1$, against the configurations $C$ in lexicographical order. The empty circles mark the $2^6 = 64$ ground-state configurations, which turn out to be the most probable (after [112]).

odically ordered region near the surface from a steady state of density fluctuations in the bulk.

This happens as follows: when the shaking energy $\Gamma$ is such that it does not distinguish between a very small void $h_n$ and the strict absence of one, the site $n$ ‘looks like’ a point of perfect packing. The grain at depth $n$ then has the freedom to point the ‘wrong’ way; we call such sites *excitations*, using the thermal analogy. The probability of observing an excitation at site $n$ scales as $\Pi(n) \approx \exp(-2|h_n|/\Gamma)$; the sites $n$ so that $|h_n| \sim \Gamma \ll 1$ will be preferred and thus dominate the low-temperature dynamics. These preferred sites are such that $n \Omega$ is closest to an integer, making them look most like points of perfect packing; misalignment vis-a-vis (3) thus costs the least. The uppermost excitation is propagated ballistically (cf. zero-temperature irrational $\varepsilon$ dynamics) until another excitation is nucleated above it; its instantaneous position $N(t)$ denotes the layer at which shape effects are lost in thermal noise, i.e., it separates an upper region of quasiperiodic ordering from a lower region of density fluctuations (5).

Fig. 4 shows a typical sawtooth plot of the instantaneous depth $N(t)$, for a temperature $\Gamma = 0.003$. The *ordering length*, defined as $\langle N \rangle$, is expected to diverge at low temperature, as excitations become more and more rare; we find in fact [112] a divergence of the ordering length at low temperature of the form $\langle N \rangle \sim 1/(\Gamma|\ln \Gamma|)$. This length is a kind of finite-temperature equivalent of the ‘zero-temperature’ length $\xi_{\text{dyn}}$, as it divides an ordered boundary layer from a lower (bulk) disordered region. Within each
of these boundary layers, the relaxation is fast, and based on single-particle relaxation, i.e., individual particles attaining their positions of optimal local packing \cite{7,9}. The slow dynamics of cooperative relaxation only sets in for lengths beyond these, when the lengths over which packing needs to be optimised become non-local.

Figure 4. Plot of the instantaneous depth $N(t)$ of the ordered layer, for $\varepsilon = \Phi$ (the golden mean) and $\Gamma = 0.003$. Dashed lines: leading nucleation sites given by Fibonacci numbers (bottom to top: $F_{11} = 89$, $F_{12} = 144$, $F_{13} = 233$) (after \cite{1,2}).

5. Discussion

In this work, we have tried to explain why jagged grains (such as would be found in gravel) pack better than smooth ones (such as bricks), when submitted to gentle shaking. Our control parameter is $\varepsilon$, the void space wasted by the disordered orientation of a grain; we have shown that irrational and rational values of this parameter lead to very different effects.

The ground state of jagged grains (irrational $\varepsilon$) is unique and only quasiperiodically ordered; that for smooth grains (rational $\varepsilon$) is highly degenerate and perfectly ordered. This is intuitively obvious; the many rough edges of irregular grains need very special orientations to click into a perfect packing, whereas rectangular bricks, for example, can be arranged in many ways so that they are perfectly packed.

The very perfection of the ground states for regularly shaped grains makes them impossible to retrieve stochastically, even in the limit of zero-temperature dynamics; instead, the effect of the latter is to give rise to density fluctuations, as predicted by our model,
and observed experimentally \[12\]. The ‘rough-and-ready’ nature of the ground state of jagged grains is by contrast quickly (ballistically) retrievable. Clearly, a sharp distinction between neighbouring rational and irrational values of $\varepsilon$ only makes sense for an infinitely deep system; for a finite column made of $N$ grains, the distinction is rounded off by finite-size effects. In particular, the characteristic features of any ‘large’ rational $\varepsilon$ are no longer observed when the period $p + q$ becomes larger than $N$.

The density fluctuations seen in the case of regular grains have a slightly non-Gaussian nature \[8\] caused by their (anti)correlations; this is reminiscent of dynamical heterogeneities in strongly compacted granular media \[13\], as well as temporal anticorrelations in cages \[14\]. Also, while the macroscopic entropy \[17\] of visited configurations in the steady state of density fluctuations is consistent with Edwards’ ‘flatness’ hypothesis \[15\], the microscopic configurational landscape is very rugged, with the most visited configurations corresponding to the ground states - as might be expected for compaction in the jamming limit. Lastly, the low-temperature dynamics for irrational $\varepsilon$ leads to an intermittency of the boundary layer separating quasiperiodic order from disordered density fluctuations; for shaking at sufficiently low intensities, it should be possible to test our detailed predictions \[1,2\] for intermittency using irregularly shaped grains.

Remarkably, many of the above features were obtained at a qualitative level in the glassy regime of a much simpler model \[7\]. On the one hand, this allows us to speculate that the shape-dependent ageing phenomena seen there could be retrieved here, i.e., that conventional ageing phenomena would only be seen for irregular grains (irrational $\varepsilon$). On the other hand, it is tempting to ask if the directional causality of the dynamical interactions present in this model and the earlier one \[7\], could be responsible for their qualitative similarity, and thus be a necessary ingredient for modelling ‘glassiness’?

Acknowledgements

AM warmly acknowledges the hospitality of the Service de Physique Théorique, Saclay, where most of this work was conceived.

REFERENCES

1. A. Mehta and J.M. Luck, J. Phys. A 36, L365 (2003).
2. J.M. Luck and A. Mehta, Eur. Phys. J. B 35, 399 (2003).
3. M. Mézard, G. Parisi, and M.A. Virasoro, Spin Glass Theory and Beyond (World Scientific, Singapore, 1987).
4. S.F. Edwards, in Granular Matter: An Interdisciplinary Approach, ed. A. Mehta (Springer, New York, 1994).
5. P.G. de Gennes, Rev. Mod. Phys. 71, S374 (1999).
6. E. Marinari, G. Parisi, F. Ricci-Tersenghi, and F. Zuliani, J. Phys. A 34, 383 (2001); M. Mézard, Physica A 306, 25 (2002); G. Biroli and M. Mézard, Phys. Rev. Lett. 88, 025501 (2002); A. Lawlor, D. Reagan, G.D. McCullagh, P. De Gregorio, P. Tartaglia, and K.A. Dawson, Phys. Rev. Lett. 89, 245503 (2002).
7. P.F. Stadler, J.M. Luck, and A. Mehta, Europhys. Lett. 57, 46 (2002); P.F. Stadler, A. Mehta, and J.M. Luck, Adv. Complex Systems 4, 429 (2001).
8. E.R. Nowak, A. Grushin, A.C.B. Barnum, and M.B. Weissman, Phys. Rev. E 63, 020301 (2001).
9. J. Berg and A. Mehta, Europhys. Lett. 56, 784 (2001); Phys. Rev. E 65, 031305 (2002).
10. J.D. Bernal, Proc. R. Soc. London A 280, 299 (1964).
11. R.L. Brown and J.C. Richards, Principles of Powder Mechanics (Pergamon, Oxford, 1970).
12. E.R. Nowak, J.B. Knight, M. Povinelli, H.M. Jaeger, and S.R. Nagel, Powder Technology 94, 79 (1997); E.R. Nowak, J.B. Knight, E. Ben-Naim, H.M. Jaeger, and S.R. Nagel, Phys. Rev. E 57, 1971 (1998).
13. A. Mehta and G.C. Barker, Phys. Rev. Lett. 67, 394 (1991); G.C. Barker and A. Mehta, Phys. Rev. A 45, 3435 (1992); Phys. Rev. E 47, 184 (1993); A. Mehta and G.C. Barker, Europhys. Lett. 27, 501 (1994); J. Phys. Cond. Matt. 12, 6619 (2000).
14. E.R. Weeks and D.A. Weitz, Chem. Phys. 284, 361 (2002).
15. S.F. Edwards, in Challenges in Granular Physics, eds. T.C. Halsey and A. Mehta (World Scientific, Singapore, 2003).
16. E. Clément and A. Lindner, private communication.
17. R. Monasson and O. Pouliquen, Physica A 236, 395 (1997).