We investigate the spatial dependence of the density of vibrated granular beds, using simulations based on a hybrid Monte Carlo algorithm. We find that the initial consolidation is typically inhomogeneous, both in the presence of a constant shaking intensity and when the granular bed is submitted to ‘annealed shaking’. We also present a theoretical model which explains such inhomogeneous relaxation in terms of a ‘consolidation wave’, in good qualitative agreement with our simulations. Our results are also in qualitative agreement with recent experiments.

I. INTRODUCTION

In recent years the issue of compaction in granular media has attracted experimental ([1], [2], [3]) as well as theoretical ([4], [5], [6], [7], [8], [9]), interest in the physics community. In particular the important issue of compactivity [10], as an effective temperature for powders in the quasi-static regime, has intrigued researchers [3] who have sought, as a consequence, to investigate further the implications of such a definition.

While this effective temperature was originally defined in terms of thermodynamic analogies for a static powder, some inconsistencies [10] have motivated work on other possible definitions. A Langevin dynamics approach, used to model vibrated powders [11], was able to introduce the compactivity as the natural interpolation of the conventional ‘granular temperature’ [2] as the intensity of vibration was decreased; this led to its interpretation as the effective temperature corresponding to the slow dynamical modes of the system. This interpretation of the compactivity was recently reformulated at a more microscopic level, in terms of a p-spin model of granular dynamics [13].

As the compactivity parameter is closely related to density variations [2], recent experimental investigations have focused on spatiotemporal density fluctuations in a shaken powder [1]. Recent molecular dynamics simulations [14] have also highlighted this issue by focusing on the necessarily inhomogeneous density fluctuations which arise when a granular system is forced by the motion of its boundaries. In this paper, we examine two aspects of spatial inhomogeneities:

• First, we examine spatial density fluctuations in the presence of a constant shaking intensity, and find definite evidence of inhomogeneous relaxation at least at short times. Additionally, as in experiment, [1], our simulations suggest that the degree of inhomogeneity is less at higher intensities of shaking. We put our observations into perspective by suggesting that the density of a vibrated granular bed initially relaxes by the propagation of a ‘consolidation wave’; this behaviour can be represented by a theoretical model that is in good qualitative agreement with our simulations.

• Second, we examine the response of the granular bed to an ‘annealed shaking’ procedure [2]; the consolidation along the so-called reversible branch of the compaction curve shows evidence of strong spatial inhomogeneities, which we demonstrate via the configurational histories of the particles. Compaction proceeds from the walls, and propagates like a consolidation wave; this is reminiscent of earlier studies of transitions to crystallinity [16] in shaken granular beds, and has also been observed in a recent experiment [17] on the appearance of ‘nematic’ ordering in an assembly of rods.

II. PROCEDURE; THE HYBRID MONTE CARLO MODEL

Our simulations use uniform hard spheres, subjected to non-sequential reorganizations which represent the effect of shaking. A variable shaking amplitude \( A \) is parametrised in units of the particle diameter; thus for example, \( A = 1.0 \) means that shaken particles are able to move longitudinally and laterally by 1 particle diameter (subject to volume exclusions) during a shake cycle. The details of the shaking algorithm have been discussed elsewhere ([7], [14]). Briefly, one cycle of vibration of the granular assembly (corresponding to one timestep of our simulation) is modelled by:

1. a vertical dilation of the granular bed, in proportion to the shaking amplitude \( A \)
2. a stochastic rearrangement of the individual particles in an external field and with available free volume proportional to the shaking amplitude
3. and finally a cooperative recompression of the assembly as each grain lands on the substrate alone or with neighbours (in the latter case, arches could form).

This algorithm has both static and dynamic disorder. The former is incorporated via the non-lattice-based nature of the simulations, while the latter is a consequence of the stochastic step, which allows particles the freedom to move in planes perpendicular to the direction of vibration, in proportion to the driving force. Collective structures, such as arches, are also allowed to form and propagate, because of the inclusion of the cooperative recompression step. In the absence of this step, particles would land sequentially, and the configurations would include only simple three-point stability conditions.

III. RESULTS ON SPATIAL DEPENDENCE OF PACKING FRACTION

In this section, we explore first numerically and then analytically, the spatial dependence of the packing fraction $\phi$ of a shaken powder. We were guided in our investigations by the knowledge that typically, experiments rely on indirect knowledge of spatial variations of material properties, since the use of 3d techniques, such as MRI \[16\], to make quantitative measurements, is still not very widespread. Consequently, we look at macroscopic quantities such as the average packing fraction $<\phi>$ and the mean particle height $Z(t)$, and extract information on spatial inhomogeneities of $<\phi>$, indirectly. In the analytical section we discuss related issues, once again from a macroscopic point of view.

A. Numerical simulations

In Fig. \[1\] we have plotted the mean packing fraction $<\phi(t)>$ against time $t$ for two different amplitudes $A$, where the angular brackets indicate an ensemble average over distinct realizations (independent sequences of pseudo-random numbers) of the noise.

![Fig. 1: Plot of mean volume fraction $<\phi(t)>$ against time $t$ for two different shaking amplitudes $A$. The open circles correspond to $A = 0.05$, while the crosses correspond to $A = 0.5$.](image)

The mean volume fraction, $<\phi(t)>$, is evaluated over the central 80 per cent of the vertical extent of the particle assembly. This central zone is defined by two planes, with heights $h_0 = 0.2Z$, $h_1 = 1.8Z$, placed symmetrically about the (volume weighted) mean particle height $Z(t)$. The granular medium is in a box with a hard base, which has periodic boundaries in the lateral directions. While all our simulations are initiated from stable loose packings with $\phi \approx 0.54$, we note that the rate of structural relaxation increases with the shaking amplitude; the time required to reach the steady state decreases with increasing $A$. More importantly however, we note that the bulk of the relaxation to the higher packing fractions occurs for the lower shaking amplitude, which is a direct consequence \[7\] of the predominance of the slow dynamics of cooperative relaxation. In this dynamical regime, collective structures remain long-standing (their autocorrelation functions decay only very slowly), and it is possible to show via the use of displacement-displacement correlation functions \[8\] that particles move together in dynamical clusters; the enhanced compaction occurs when the net void space trapped in these clusters is shaved off.

![Fig. 2: Plot of mean particle height $Z(t)$ against time $t$ for two different shaking amplitudes $A$. The open circles correspond to $A = 0.05$, while the crosses correspond to $A = 0.5$.](image)

In Fig. \[2\] we plot the mean particle height $Z(t)$ against time $t$; this is an important indicator of consolidation as it shows the average distance of the particles from the base. We notice that the final value of $<Z(t)>$ is smaller for smaller shaking amplitudes. In other words, the particles are more efficiently settled or ‘sedimented’ for gentler shaking, and consolidation is thus stronger.

These two indicators are independent measures of consolidation, but reveal nothing about its nature. Their product $<Z(t)\phi(t)>$, however, provides an insight into whether the consolidation is homogeneous or inhomogeneous; this is plotted in Figure \[3\].
Consider the simplest form of inhomogeneous consolidation, i.e. the volume fraction changes discontinuously from an initial uniform density, $\phi_0$, to a maximum density, $\phi_{\text{max}}$, at each layer of a (three-dimensional) vibrated granular bed, following the passage of a 'consolidation wave'. We visualise the process of consolidation to be analogous to that which is known to occur in sedimentation, when particles settle onto a sediment at the bottom of a particulate suspension. In this way, we imagine that shaken grains settle to the bottom of the vibrated bed in a more compacted state than they were previously, and that this settling defines the position of the front of the consolidation wave.

Let $z_{\text{max}}(t)$ be the position of the highest layer with density $\phi_{\text{max}}$ at time $t$; this then defines the position of the front of the consolidation wave. Let $z_0(t)$ be the position of the upper surface (characterised by a density $\phi_0(t)$ at time $t$). Assuming that consolidation is uniform in the plane perpendicular to the direction of vibration (which we choose to be the $z$-direction), while it is inhomogeneous in the direction of vibration, conservation of mass gives

$$\phi_{\text{max}}(t) z_{\text{max}}(t) + \phi_0(t) (z_0(t) - z_{\text{max}}(t)) = \phi_0(0) z_0(0)$$  \hspace{1cm} (1)

The position $Z(t)$ corresponding to the mean particle height at time $t$ is:

$$Z(t) = [(\phi_{\text{max}}(t) - \phi_0(t)) z_{\text{max}}(t)]^2 + \phi_0(t) z_0(t)^2 / 2 \phi_0(0) z_0(0)$$ \hspace{1cm} (2)

The position of the consolidation wavefront $z_{\text{max}}(t)$ relative to the central zone, i.e. the region between planes $h_0(t) = 0.2Z(t)$ and $h_1(t) = 0.8Z(t)$, defines the measured mean volume fraction $< \phi(t) >$ at time $t$:

$$< \phi(t) > = \phi(0) \quad z_{\text{max}}(t) - h_0(t)$$ \hspace{1cm} (3)

$$< \phi(t) > = (\phi_{\text{max}} - \phi_0) z_{\text{max}}(t) + (1.8\phi_0 - 0.2\phi_{\text{max}}) Z(t))/1.6Z(t)$$ \hspace{1cm} (4)

$$9h_0(t) > z_{\text{max}}(t) - h_0(t)$$ \hspace{1cm} (5)

Equations (2) and (3) give in qualitative agreement with Figures 2 and 3.

In order to explain the non-trivial behaviour of the product $< \phi(t)Z(t) >$, we note that at large times, $t \rightarrow \infty$, we must have:

$$z_{\text{max}}(t) = z_0(t) = 2Z(t)$$ \hspace{1cm} (6)

$$\phi_{\text{max}} Z(t) = \phi(0) Z(0)$$ \hspace{1cm} (7)

since the consolidation wavefront will have reached the upper surface at large times. Then, using the above equations, and simplifying, we find that for short times, the normalized product $< \phi(t)Z(t) >$ (which approaches one as $t \rightarrow \infty$), is given by

$$[\phi(t)Z(t)]/[\phi_{\text{max}} Z(\infty)] = Z(t)/Z(0)$$

$$= z_0(t)/z_0(0) + ((\phi(0)/(\phi_{\text{max}} - \phi_0))( [ (z_0(0) - z_0(t))/z_0(0)]^2) \hspace{1cm} (8)

The first term on the right-hand-side is expected to be less than one in the case of consolidation, since the height of the upper surface should decrease with time as the granular bed compacts. The second term, in this case, is also clearly positive; its size, however, depends on the size of the coefficient $\phi(0)/(\phi_{\text{max}} - \phi(0))$. We have seen in Figure 1 that small values of $\phi_{\text{max}} - \phi(0)$ correspond to large shaking amplitudes $A$, and conversely. This results implies, in agreement with earlier work on compaction, that the overall consolidation is larger for lower shaking amplitudes. Thus, for large $A$ the normalised product $< \phi(t)Z(t) >$ can be greater than one; for small shaking amplitudes, on the other hand, the value of the product can be less than one (the value of $\phi(0)/(\phi_{\text{max}} - \phi(0))$ is small). These results obtained in the short-time limit of this very simple model, are in excellent agreement with the results of the simulation (Figure 3).
IV. IRREVERSIBLE AND REVERSIBLE BRANCHES IN ANNEALED SHAKING: MORE CONSOLIDATION WAVES

Recent explorations of compaction in a shaken powder have involved the analogue of ’annealed cooling’ [2]: a granular bed, prepared at very low density, is subjected to $t_{tap}$ taps at intensity $\Gamma$; the intensity is then incremented in steps of $\delta \Gamma$. This results in a compaction curve with two branches; an irreversible branch, where increasing the tapping intensity leads to increasing packing fractions, and a (so-called) reversible branch, where the reverse is the case. We have simulated the ’annealed shaking’ of a granular bed of 1300 particles for 1425 shakes, such that $\delta \Gamma = 1/500$ and $t_{tap} = 1$, corresponding to a continuous variation of shaking intensity. As before, there is a hard base in the lower $z$ direction, while there are periodic boundary conditions in the $x$ and $y$ directions. The intensity is increased from $A = 0.05$ to $A = 1.0$, decreased to $A = 0.05$ and increased back again to $A = 1.0$.

Our results (Fig. 4) show that the packing fraction first increases from 0.55 along the irreversible branch before decreasing at high values of $A$; it then increases as $A$ is reduced along the so-called reversible branch. Any further changes of shaking intensity cause it to remain on this branch, except for a small hysteresis loop; the presence of this hysteresis loop indicates that even the so-called reversible branch is irreversible in reality. We expect that the size of this hysteresis loop would increase for large $\delta \Gamma$ and small $t_{tap}$, and conversely; the irreversibility of the ’reversible’ branch consequently mirrors the degree of irreversibility of the annealed shaking process.

FIG. 4. Plot of packing fraction $\phi$ vs shaking intensity $A$ for the annealed shaking of a granular bed. Note the hysteresis loop in the ’reversible branch’, showing a fundamental irreversibility.

In order to look more microscopically at what occurs along both branches of the compaction curve, we present in Fig. 5 snapshots of the configurations of the spheres. Each snapshot corresponds to a distinct value of the shake intensity $A$ as the compaction curves of Fig. 4 are swept. The first three configurations correspond to $A$ increasing on the irreversible branch, the second three, to $A$ decreasing on the reversible branch, and the last three to $A$ increasing along the reversible branch. We note, especially along the ’reversible’ trajectories that a ’crystalline’-like ordering appears to spread from the base as the shake intensity is continuously decreased, which has a wavelike character. The presence of this ’consolidation wave’ mirrors a recent experimental result, where ordering in an assembly of rods is seen to originate at the walls and to propagates like a wavefront [17].

FIG. 5. Configurations for selected evenly spaced shaking amplitudes $A$, a) on the irreversible branch $A = 0.3, 0.6, 0.9$, b) the ’reversible’ branch for $A$ decreasing $A = 0.8, 0.5, 0.2$, and finally c) the ’reversible’ branch for $A$ increasing $A = 0.15, 0.45, 0.75$

Investigations are under way to analyse these structures further, with the use of appropriate order parameters [20] in the context of an observed crystallisation transition in shaken granular beds [16].

V. DISCUSSION

We have presented a simple model of short time inhomogeneous consolidation, based on the idea of a consolidation wave; its analytical solution is in good agreement with our
Monte Carlo simulations of vibrated (three-dimensional) particle packings. Despite the simplicity of our model, it manifests an important signature of inhomogeneous consolidation for early and intermediate times, in agreement with the simulations. Interestingly these are both in agreement with experimental data [1], where it was shown that the larger the intensity of vibration, the more homogeneous the consolidation; notice that the data for the larger vibrational intensity asymptote much more quickly (Figure 3). Investigations are in progress to look in greater detail at the local structures in the particle packings, and at the detailed spatial variations inherent in the inhomogeneous packings [2]. Ongoing work also includes a detailed investigation of inhomogeneous density fluctuations in a vibrated powder, and their repercussions for its power spectrum [2].

Additionally, we have presented ancillary evidence for consolidation waves via the study of particulate configurations in the annealed shaking of a granular bed. In addition to the aspects on which we have reported here, an analytical study of a simple lattice-based model [2] of a shaken granular bed is expected to yield valuable insights on the precise influence of spatial inhomogeneities along the reversible and irreversible branches of the compaction curves.

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