Effect of Rare Events on Out-of-Equilibrium Relaxation

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This Letter reports experimental and numerical results on particle dynamics in an out-of-equilibrium granular medium. We observed two distinct types of grain motion: the well known cage motion, during which a grain is always surrounded by the same neighbors, and low probability “jumps,” during which a grain moves significantly more relative to the others. These observations are similar to the results obtained for other out-of-equilibrium systems (glasses, colloidal systems, etc.). Although such jumps are extremely rare, by inhibiting them in numerical simulations we demonstrate that they play a significant role in the relaxation of out-of-equilibrium systems.

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Glasses, colloids, and granular materials are characterized by structural disorder at the mesoscopic scale. These heterogeneous and metastable systems share a number of dynamical properties, such as aging and slow relaxation, in which the cage motion of individual grains plays a significant role. Many experimental and numerical efforts have been made to observe and understand the out-of-equilibrium behavior exhibited by these systems [1–8]. A full understanding of the macroscopic behaviors of these systems requires detailed observations at the local scale (i.e., at the scale of a particle). The local dynamics in glasses is numerically simulated with Lennard-Jones liquids, and the motion of atoms can be correlated to the α and β relaxation regimes [6]. Similar observations are obtained experimentally on colloidal systems using confocal microscopy [4], granular media in 2D [3], or 3D granular assemblies immersed in index matching fluid [7]. For all these systems, the cage effect is clearly identified. Here we present an extensive experimental and numerical study of particle motion in 3D granular packing under gentle vertical tapping. Although this system is not thermal (its thermal energy is irrelevant in comparison with the energy needed to move a macroscopic grain), it is often presented as an ideal system to study out-of-equilibrium systems. From a microscopic point of view, this analogy is based on the idea that the geometry of the grains plays a major role, similar to geometrical frustration in thermal glasses. Indeed, like glasses, a granular assembly can be trapped in a metastable configuration unless an external perturbation such as shear or vibration is applied. Note that, unlike thermal energy, mechanical agitation of grains is, in general, neither stochastic nor isotropic. We expect, as others have found [2,3,7,9–12], that the results obtained are valid for any of the above mentioned out-of-equilibrium systems. Let us recall that, when a dense granular sample is submitted to gentle external mechanical perturbations, its packing fraction Φ increases quickly at the beginning, then gradually approaches an asymptotic value. This slow compaction is similar to the slow dynamics observed in other out-of-equilibrium systems [2,10,13].

The experimental results presented in the first part of this Letter are obtained with D = 0.6 mm diameter glass spheres placed in a glass cylinder of diameter 6 mm. This container is placed on a plate connected to an electromagnetic exciter. The glass spheres are immersed in index matching oil containing a laser dye. When imaged from the objective lens through the bottom of the sample container, beads appear as dark circles. Sequences of 10^4 taps are carried out. The only control parameter is the tapping intensity Γ = γ_max/g, where g = 9.81 m·s^-2 and γ_max is the maximum of the acceleration monitored by the accelerometer when the plate goes down [14]. It should be pointed out that we used only taps for which the grains took off from the bottom of the glass cylinder, i.e., above the lift-off threshold. Results from numerical simulations are shown in the second part of this Letter. In these simulations, the compaction of 4096 monosize spheres of radius R under tapping from a low packing state to a higher one is studied. The container is a box with a flat 32R X 32R square bottom with periodic boundary conditions imposed in the horizontal directions and a free interface at the top of the packing. A tap is simulated in two stages. First, the packing is dilated vertically according to the law \( z - R \rightarrow (z - R)(1 + \varepsilon) \), where \( \varepsilon \) is the dilation parameter. This dilation increases the free volume and allows for the reorganization of beads. This linear behavior during a tap is also observed in our experiments, and the parameter \( \varepsilon \) is proportional to the square of the experimental parameter Γ [15]. The second stage simulates the gravitational redeposition, with a nonsequential algorithm [16] in order to observe the collective behavior. The model takes only the steric constraints into account, which are fundamental for the compaction. While the simulation does not calculate the stress transmission in the packing, it describes rela-
tively accurately the grain motion during a tap [17], contrari
to other simulations such as the Tetris model, for
example, which show slow relaxation and aging but whose
dynamics have no direct relation with particle motion.
Finally, our simulation results closely match the experi-
mental results. The experimental setup and the numerical
simulation are described in detail in Refs. [10,16].

During an experiment in index matching fluid, cage
motion and jumps were observed. The cage motion is
always characterized by the fact that a grain is always
surrounded by the same neighbors. A jump is a displace-
ment during which a grain moves significantly more than
the mean displacement of a grain. Such an event observed
by confocal microscopy is shown in Fig. 1. The horizontal
cross sections shown were taken during the same exper-
iment, at the same height in the medium for two successive
taps (125th and 126th). On each picture, two different
layers of the granular medium are visible. The beads of
the lower layer have a well-defined black outline and a
bright central part, and the beads belonging to the upper
layer are black. The vertical position of a bead is deter-
dined by measuring its apparent radius in the picture.
Since the beads move only a small fraction of a bead
diameter between taps, it is possible to track their positions
from frame to frame. A rare occurrence of jump is indi-
cated by an arrow in Fig. 1. This bead, during a tap, has
fallen from the upper visible layer to the lower one by a
displacement larger than all the others. The amplitude of
this jump between the two layers is $0.388D$ compared to
the mean displacement in a layer, which is $0.00216D$, as
shown in the distribution of bead displacement reported in
Fig. 1.

The study of the grain motion during our simulation
confirms that the displacement of the beads exhibits two
different scales. The smaller scale corresponds to the cage
motion during which a grain explores the trap created by its
neighbors. Previous results [3,6] demonstrate the non-
Gaussian character of the displacement distribution ob-
tained in a 2D experiment and glass media, respectively.
Such non-Gaussian behavior is also observed in our ex-
perimental and numerical systems. Figure 2 shows the
histogram of displacements in the $x$ direction and the
corresponding Gaussian fits. Deviations from the fits can
be observed in the tails of the distributions. Note that the
deviation is more important for the numerical simulations.
The characteristics of the cage motion change during the
simulation, because of the evolution of the packing frac-
tion. Indeed, the average magnitude of this displacement
decreases with the decrease of the void space in the me-
dium. The larger scale corresponds to a jump: a very low
probability event during which a bead enlarges its trap and,
thus, escapes from it. Figure 3 shows the trajectory of a
bead which is subject to a “jump” during the 100 first taps
in the simulation. The initial drift in position is due to the
increase of the packing fraction and, consequently, to the
decrease of the sample height. At the 46th tap, the bead
displacement is $0.48D$, although the average displacement
(apart from the jump) is $0.0038D$. We found that the jumps
always yield a large displacement in the direction of grav-
ity, as they are correlated to the compaction mechanism
and correspond to the fall of a bead in a hole located under
it. Note that the magnitudes of the cage motion and of the
jumps are both of the same order in simulations and experi-

![FIG. 1 (color online). Experimental observation of a jump and
distribution of bead displacements obtained by confocal imaging
in an index matching fluid. The two pictures correspond to a
horizontal cross section at the same altitude of the granular
sample before and after the 126th tap of intensity $\Gamma = 6$. All
the beads remain in their original layer except one bead (pointed
out by a white arrow) which falls from the upper to the lower
layer. The distribution of bead displacements computed for
10 taps, 5 before and 5 after the 126th tap, reveals the two scales
of displacement.](image1)

![FIG. 2 (color online). The histogram of displacements in a
horizontal direction ($\delta x$) for our 3D experiment ($\Gamma = 6$) and for
our corresponding numerical simulation ($\varepsilon = 0.05$). The lines
correspond to Gaussian fits. We observe deviations from the fits
in the tails of the distributions.](image2)
moves down, and if its displacement vertical displacement of a bead is negative, i.e., if the bead jumps, the following test is added to the algorithm: If the jumps and with inhibited jumps are compared. To avoid inhibited in the simulation, and the evolutions with normal jump is possible only if the hole is large enough. mainly at the beginning of the simulation, when the pack-

diodecaying function the probability of acceptance follows an exponentially displacement is not accepted with probability 1. Instead, the mean displacement of beads in the layer $h$ can be interpreted as two states that are separated by high jumps than with jumps. In terms of energy landscape, this obtained after a large number of taps is less dense without jumps. The simulation, thus, correctly represents both the local and global behaviors of the granular material. The jumps are extremely rare events and, therefore, are difficult to observe experimentally. In a simulation of 10 000 taps for $N = 4096$ beads, only about 100 jumps occurred, mainly at the beginning of the simulation, when the packing fraction is still far from the steady state value. Indeed, a jump is possible only if the hole is large enough.

To understand the importance of the jumps, they are inhibited in the simulation, and the evolutions with normal jumps and with inhibited jumps are compared. To avoid jumps, the following test is added to the algorithm: If the vertical displacement of a bead is negative, i.e., if the bead moves down, and if its displacement $d_i$ is larger than twice the mean displacement of beads in the layer $\langle d \rangle$, this displacement is not accepted with probability 1. Instead, the probability of acceptance follows an exponentially decreasing function $\exp(- (d_i - 2 \langle d \rangle)/\delta)$. The brackets $\langle \rangle$ denote the average over a layer, and $\delta$ is calculated such that the probability is $10^{-6}$ when $d_i = R$ (the radius of a bead). Note that we checked with a molecular dynamics simulation that prohibiting jumps does not lead to mechanically unstable packings. The evolution of the packing fraction during the simulation with jumps and with strongly inhibited jumps is shown in Fig. 4. This graph reveals that, without significant jumps, the increase of packing fraction during the initial evolution is slower. This seems to make sense as some large displacements do not occur in this case. But, surprisingly, the packing obtained after a large number of taps is less dense without jumps than with jumps. In terms of energy landscape, this can be interpreted as two states that are separated by high potential barriers that cannot be circumnavigated by many slow events, and we can conclude that the energy landscape exploration is completely different without jumps. Although jumps are extremely rare events, they play a significant role in the evolution of the media. As we have noted earlier, the number of these events decreases as the system compacts, and the great majority of jumps happens during the first 250 taps. So the initial behavior determines the subsequent evolution. Somewhat similar to the well known memory effects reported first in Ref. [9], the medium never completely forgets its initial evolution. To have better insight into the effect of jumps, we study the evolution of $\langle \Delta r^2(t) \rangle = \langle (r(t) - r(0))^2 \rangle$, where $r(t)$ is the grain position at time (i.e., number of taps) $t$, with and without jumps. The brackets $\langle \rangle$ denote the average over the grains. The results are reported in Fig. 5 for a dilation parameter $\varepsilon = 0.05$. In the two cases, a subdiffusive behavior is found. Note that it is not possible to compare directly the two evolutions, since the packing fractions are not the same with jumps or with inhibited jumps. A modified random walk model that mimics the cage motion can, nevertheless, shed new light on the diffusive properties without jumps, where cage motion is the only allowed displacement. Two main characteristics were introduced in this model. First, an increase in packing fraction (thus, a decrease in cage size) results in decreased mean grain displacements. Second, the high anticorrelation of the motion inside a cage: Since the cage is a closed space, the probability to have at time $t$ a step in the opposite direction of the step at time $t-1$ is higher than the probability to have these two steps in the same direction. A 3D random walk is then generated for 4096 walkers. The step magnitude is chosen to fit the decrease of the void in the sample: $d_i = \alpha (\Phi(t)^{-1} - 1)^{1/3}$. The fitting parameter $\alpha$ is adjusted to
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We have studied experimentally and numerically the bead motion during compaction of a granular medium. We have demonstrated that extremely rare "microscopic" events (jumps) have huge consequences on the "macroscopic" behavior: Simulations show that compaction is slower and that the state reached after many taps is less dense if the jumps are "inhibited." This result is important and surprising because, in an equilibrium system, such rare events have negligible effects on its overall evolution. Such results, obtained for an out-of-equilibrium granular medium, should also be valid for other out-of-equilibrium systems (glasses, colloids, etc.) and could be useful for the study of segregation of granular mixtures under shearing [19].

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FIG. 5 (color online). Evolution of $\langle \Delta r^2 \rangle$ with $t$ for simulations with jumps and with inhibited jumps but for the same dilation parameter $\varepsilon = 0.05$. The random walk created correctly describes the behavior without jumps but fails to reproduce the behavior observed with jumps.

have the same mean displacement in the numerical simulation and in the random walk. Finally, the direction of the step is chosen as follows: The azimuthal angle $\theta(t)$ is chosen uniformly between 0 and $2\pi$ and the polar angle is given by $\varphi(t) = \pi - \varphi(t - 1) + \eta$, where $\eta$ is a Gaussian noise of average zero and of variance $\pi(\Phi_{\text{max}} - \Phi)/(\Phi_{\text{max}} - \Phi_0)$. The values $\Phi_0$ and $\Phi_{\text{max}}$ are, respectively, the initial value of the packing fraction ($t = 0$) and the packing fraction obtained at the end of the simulation (averaged between $t = 9900$ and $t = 10000$). This decrease of the variance mimics the increase of anticorrelation with the increase in packing fraction $\Phi$. We have reported in Fig. 5 $\langle (r(t) - r(0))^2 \rangle$ obtained by the random walk model using the fit parameter $\alpha$ corresponding, respectively, to the data with jumps and with inhibited jumps. This random walk describes correctly the evolution of $\langle (r(t) - r(0))^2 \rangle$ without jumps, as expected, but fails to describe the behavior with jumps. The initial evolution is too slow, as shown in the inset in Fig. 5, and the final evolution shows correlations which are too weak to describe the bead motion. The creation of a void large enough to allow a jump requires not only the motion of the first neighbors but also the motion of a large cluster [18]. Consequently, although the jumps are low probability events, they affect the motion of all the beads, and, thus, the dynamics with jumps corresponds to more complex mechanisms.

We have studied experimentally and numerically the bead motion during compaction of a granular medium. We have demonstrated that extremely rare "microscopic" events (jumps) have huge consequences on the "macroscopic" behavior: Simulations show that compaction is slower and that the state reached after many taps is less dense if the jumps are "inhibited." This result is important and surprising because, in an equilibrium system, such rare events have negligible effects on its overall evolution. Such results, obtained for an out-of-equilibrium granular medium, should also be valid for other out-of-equilibrium systems (glasses, colloids, etc.) and could be useful for the study of segregation of granular mixtures under shearing [19].

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