Rattler-induced aging dynamics in jammed granular systems

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Granular materials jam when developing a network of contact forces able to resist the applied stresses. Through numerical simulations of the dynamics of the jamming process, we show that the jamming transition does not occur when the kinetic energy vanishes. Rather, as the system jams, the kinetic energy becomes dominated by rattlers particles, that scatter withing their cages. The relaxation of the kinetic energy in the jammed configuration exhibits a double power-law decay, which we interpret in terms of the interplay between backbone and rattlers particles.

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I. INTRODUCTION

The solid to liquid transition of granular systems, beside controlling many natural phenomena such as earthquakes or landslides, is of great theoretical interest since it is related to an out-of-equilibrium phase transition [1–4] and to the physics of glass forming systems. The control parameters that drive this transition are the density/pressure, the shear strain/stress [1], as well as the frictional properties of the grains [8, 9]. This transition has been extensively investigated in the static limit, where the grain dynamics is either absent or negligible. For instance, the earliest investigation of the transition [10] considered the evolution of the properties of jammed packings of frictionless grains as the density approaches the critical value and a number of experimental and numerical following works have been conducted in the same spirit [11, 12]. Similarly, the shear induced transition from the jammed to the flowing state has been mainly investigated in the limit of quasistatic deformations. In numerical simulations, this limit is realized by minimizing the energy after every infinitesimal increase of the shear strain [13], which makes inertial effects irrelevant. While the quasistatic approximation is reasonable when describing the transition from the solid to the fluid state, since in the solid phase particle motion is negligible, it must be relaxed to describe the transition from the flowing to the jammed state. Indeed, inertial events make the jamming/unjamming transition hysteretic [14] by affecting the location of the transition threshold.

In this paper we numerically investigate the transition from the unjammed to the jammed state in a model system exhibiting stick-slip motion. The model consists of a collection of grains confined in between two rigid plates at constant pressure. The bottom plate is fixed, while the top one is driven through a spring mechanism, as in spring-block models, which leads to a stick-slip motion. This and similar models have been investigated by a number of authors in both experiments and simulations [12, 15, 24], that focused on the identification of slip precursors, on the study of the response to external perturbations [13, 25, 28] and on the characterization of the slip size distribution, that has been shown to be affected by inertial effects [30]. In this model, a slip starts when the granular system becomes unable to sustain the shear stress exerted by the top plate, and it ends as soon as it becomes able to balance again the shear stress whose value has decreased because of the slip. In this jammed configuration, the velocity of the top plate vanishes, and a network of contact forces between the grains counterbalance the applied stress [15]. Here we show that, surprisingly, the kinetic energy of the systems is not zero when the system jams. Rather, the kinetic energy never vanishes, but decreases in time as a power law, with a crossover between a slower decay at short times and a faster decay at long times. We show that this behavior originates from coupled structural and dynamical heterogeneities, due to the coexistence of particles forming the sustaining backbone and rattlers free to move in cages formed by the backbone particles. Indeed, the first slower relaxation regime is affected by both the backbone particles and the rattlers, while the second one is dominated by the rattlers. The crossover between the two regimes is detected at a characteristic time \( \tau_c \), depending on external constraints.

II. MODEL

We perform three-dimensional molecular dynamics simulations of the model illustrated in Fig. 1a, consisting of \( N \) monodisperse spheres of unitary mass \( m \) and diameter \( d \), enclosed between two rigid rough plates of dimension \( L_x \times L_y \). Each plate is made of \( L_xL_y/d^2 \) grains, placed in random positions in the \( xy \)-plane. The \( z \) position of these grains is randomly shifted to make the plates corrugated. The relative positions of the particles belonging to the plates are fixed in order to make the plates...
FIG. 1: (Color online) (Upper panel) Our model system consists of a collection of grains (gray particles) confined between two rough plates at constant pressure. The top plate is driven through a spring whose free end moves with a constant velocity $V_d > 0$. (Lower panel) The time evolution of the top plate position during a short time interval in which two slips occur.

rigid. The top plate is subject to a constant pressure $p$ applied along the $z$ direction and attached to a spring of elastic constant $k_m$, whose free end moves with constant velocity $V_d$ in the $x$ direction. We employ a contact force model described in [31] where particles interact along the normal direction via the standard spring-dashpot model with a restitution coefficient $e$. We measure the mass in units of $m$, the length in units of $d$ and time in units of $\sqrt{m/k_m}$. All model parameters have been chosen according to Ref. [15, 16] in order to have long stick phases interrupted by rapid plate displacements, i.e. the slips, namely: $N = 1000$, $L_x \times L_y = 20 d \times 5 d$, $p = k_m/d$, $e = 0.88$, $V_d = 0.01 d/\sqrt{m/k_m}$. Due to the constant pressure condition, the size of the system along the vertical direction is not fixed, but slightly fluctuates around $L_z \approx 10$. The majority of slips $S_i$ involve small displacements of the top plate, i.e. of the order of a small fraction of a grain diameter $S_i \ll d$, however also slips involving the whole system $S_i \sim L_x$ are observed [13, 16]. The temporal integration step of the equations of motion is $5 \times 10^{-3} \sqrt{m/k_m}$.

III. RESULTS

A. Relaxation after a slip

During a slip, the system dissipates energy and the applied stress decreases. When the slip is over, the system should be found, in principle, in a jammed state in which the top plate velocity is zero. This only occurs, however, in the limit $V_d \to 0$, since for finite $V_d$ in the jammed state the top plate exhibits a creep motion as the system continuously adapts to the increasing shear stress. Figure 1b illustrates the time evolution of the position of the top plate of our system, in a temporal window where two slips occur at time $t_{s_i}$, $i = 1, 2$. Specifically, considering that a slip has a finite duration, here we define $t_{s_i}$ as the time at which the slip ends [15], so that $t_{s_i}$ corresponds to the onset of the stick phase. We define $t_s$ as the time at which the velocity of the plate becomes smaller than a given threshold, $10^{-2}$. For $t > t_s$ the velocity of the top decreases in time while exhibiting a jerking motion. This is a consequence of the creep motion that sets in due to the increasing shear stress controlled by the

FIG. 2: (Color online) Kinetic energy relaxation of several replicas of the system with different temporal distances from two slip occurrence times $t_{s_1}$ and $t_{s_2}$. (Upper panel) The short time behavior of the energy $K(t)$ clearly depends on the value of $t - t_{s_i}$, while it is mainly $(t - t_{s})$-independent at large times. (Lower panel) Kinetic energy is plotted as a function of $\tau = t - t_s$. Data obtained for different $t - t_s$ collapse onto a single curve, exhibiting two power law regimes.
driving velocity $V_d > 0$. To investigate the relaxation dynamics following a slip without being affected by the creep motion and by subsequent slips, we investigate the jamming dynamics of replicas of the system that evolves with zero driving velocity, $V_d = 0$. We create replicas at many different times $t_c$ after the slip time $t_s$. During the relaxation dynamics the top plate of the replica performs damped oscillations and rapidly reaches a rest position, confirming the absence of creep motion.

Since the velocity of the top plate of the replica evolving with $V_d = 0$ vanishes, one might expect the system to reach a jammed state in which there is no particle motion. Conversely, the investigation of the time evolution of the kinetic energy of the replicas (Fig. 2) reveals that this is not the case. Indeed, even if the system is in a macroscopic jammed state, the decay of the kinetic energy, measured from the time of replica creation, $t - t_c$, is consistent with a power law indicating that the stationary condition $K = 0$ is never reached. The system, therefore, never attains a state of mechanical equilibrium. Fig. 2 (upper panel) shows that the kinetic energy depends on the time $t_c$ at which the replica is made, and decreases as $t_c$ increases. Conversely, data collapse when plotted as function of the time since the last slip $\tau = t - t_c$, as in the lower panel of Fig. 2. Two different regimes in the temporal decay of the kinetic energy are detected, with a crossover occurring at $\tau_c \simeq 7000$. For $\tau < \tau_c$, the kinetic energy decreases as $K \sim \tau^{-\psi_1}$, while for $\tau > \tau_c$ it decreases as $K \sim \tau^{-\psi_2}$. Averaging over 10 different slips, we estimate $\psi_1 = 1.3 \pm 0.1$ and $\psi_2 = 1.8 \pm 0.1$. Combining the two scaling regimes, we expect

$$K(\tau) = A\tau^{-\psi_1} \left( \frac{\tau}{\tau_c} + 1 \right)^{-\psi_2 + \psi_1}. \tag{1}$$

As we will describe later, this equation holds for any $\tau$ larger than a microscopic time $t_0$ and is observed for slips of different sizes with the value of $\tau_c$ and $A$ depending on the particular slip.

We next show that the observed relaxation dynamics results from the interplay between rattlers and backbone. Indeed, in our system we observe that during the relaxation dynamics a small fraction of particles, less than 10%, are located inside cages and are not in permanent contact with other particles. These are the rattlers, each of which moves in a cage of volume $\sim (1 + 10^{-3})d^3$. In Fig. 3 we evaluate the separate contribution to the kinetic energy from the backbone particles and the rattlers, for a given replica, but analogous results are found for all replicas. The figure clarifies that, despite their small number, rattlers dominate the total kinetic energy of the system. This result allows to rationalize why the kinetic energy of a replica made a time $t_c$ only depends on the time elapsed since the preceding slip, as in the lower panel of Fig. 2.

Being the kinetic energy dominated by the rattlers, this is not influenced by the creep motion, and it is therefore insensitive to the time $t_c$ at which the creep motion is suppressed by setting the driving velocity to zero. Fig. 3 also shows that the $\tau$ dependence of the kinetic energy of the backbone exhibits a clear change of behavior at the crossover time $\tau_c$, becoming much slower for $\tau > \tau_c$. This suggests a physical interpretation in which the crossover in the decay of the kinetic energy relates to the stiffening of the backbone, we describe in the following.

### B. Physical origin of the crossover

To rationalize the crossover in the decay of the kinetic energy, Eq. 1 we consider that energy is dissipated though inter-particle collisions. Let’s suppose that rattlers colliding with the backbone with typical kinetic energy $K$ lose an amount of energy scaling as $\Delta K \sim K^{1+\epsilon}$. Thus, the typical energy variation $dK$, in a time interval $dt$, is proportional to the average number of collisions $n_{dt} \propto K^{1/2}$ in $dt$ times the average energy dissipated in each collision $\Delta K$, $dK/dt \propto -n_{dt}\Delta K$. This leads to $dK/K^{3/2-\epsilon} \propto -d\tau$, so that $K \sim \tau^{\psi}$, with $\psi = \frac{2}{3+2\epsilon}$. Accordingly, the crossover in $\psi$ occurring at time $\tau_c$ should correspond to a crossover in $\epsilon$. We have explicitly checked this prediction in numerical simulations, investigating the kinetic energy lost $\Delta K = K(\tau + d\tau) - K(\tau)$ as function of $K(\tau)$, for different values of $\tau$ and a fixed small value of $d\tau$. Fig. 4 shows that $\Delta K$ does actually exhibit a crossover at $\tau_c$, scaling as $\Delta K \simeq K^{1+\epsilon}$ with $\epsilon \simeq 0.3$ for $\tau < \tau_c$, and $\epsilon \simeq 0$ for $\tau > \tau_c$. These values of $\epsilon$ are consistent with the expected values of $\psi = \frac{2}{3+2\epsilon}$.

Physically, the crossover in $\epsilon$ can be attributed to a dynamical transition of the backbone. Indeed, the crossover in the decay of the kinetic energy reported in Fig. 2 suggests that the backbone behaves as a rigid structure only for $\tau > \tau_c$. If this is the case, for $\tau > \tau_c$ rattlers move in rigid cages, and dissipate in each collision an amount...
of energy equal to $\Delta K = (1-e)K$, with $e$ the restitution coefficient, in agreement with the $\epsilon = 0$ expectation. Conversely, for $\tau < \tau_c$, rattlers are able to transfer energy to the rigid structure, so that the energy lost in a collision is larger than $(1-e)E$, which leads to a positive $\epsilon$. Summarizing, the long–time regime, $\psi = \psi_2$, is observed when cages become rigid, whereas the first short–time regime, $\psi = \psi_1$, reflects the relaxation of cages towards their stationary configuration. In this picture, the inelastic collisions with the rattlers are the main dissipation mechanisms leading to the freezing of the backbone. Thus, the time $\tau_c$ is expected to be inversely proportional to the dissipated energy.

This hypothesis leads to a relation between $\tau_c$ and the constant $A$ in Eq. 1. Indeed, considering that the energy dissipated in the interval $[t_0, \tau_c)$ scales as $A^{5/2}\tau_c$ and that $\psi_1 = \frac{1}{1+\psi_2}$, one has

$$K(\tau) \propto \tau_c^{-\alpha} G\left(\frac{\tau}{\tau_c}\right) ,$$

with $\alpha = \psi_1 + \frac{\psi_2}{1+\psi_1}$ and $G(x) = x^{-\psi_2}(x+1)^{-\psi_2+\psi_1}$.

To verify this prediction, we have investigated the relaxation of replicas created after slips of different size. As illustrated in Fig. 4 (left panel) the raw data for the relaxation dynamics of the kinetic energy (upper panel) nicely collapse when the energy and time are rescaled according to Eq. 2 (lower panel), confirming our interpretation.

In addition, we have performed simulations to better clarify the role of the rattlers in the stabilization of the backbone. Indeed, if the backbone dissipates energy and freezes mainly interacting with the rattlers, then the crossover time $\tau_c$ is expected to decrease on increasing the backbone-rattlers collision frequency. Thus, we have monitored the relaxation dynamics of the replicas, after scaling the velocity of each rattler by a factor $Q$, i.e. $v \rightarrow Qv$, keeping $Q$ small enough not to destabilize the backbone. Results, plotted in Fig. 4 for a given replica and for $Q \in [0.25, 10]$, show that $\tau_c$ decreases with $Q$, whereas $A$ increases with $Q$. In Fig. 6 (lower panel) we plot $\tau_c^2 K$ as function of $t / \tau_c$, obtaining a good data collapse for all values of $Q$ in agreement with the scaling relation Eq. 2. Analogous results are obtained for different replicas.

The above interpretation is supported by the evolution of the elastic energy $U(t)$ of the backbone particles which, during the undriven phase, presents oscillations around a constant value $U_\infty$, as illustrated in the inset of Fig. 4. The fluctuations of this elastic energy, $\sigma(t) = \sqrt{\langle (U^2(t)) - \langle U(t) \rangle^2 \rangle}$, where $\langle \cdot \rangle$ indicate temporal averages over a time scale $t_{\text{ave}} = 10$, are a proxy of the degree of stiffness of the backbone. Fig. 7 (upper panel) shows that the fluctuations of the elastic energy decays in time exhibiting a double power law, with a crossover time occurring at time $\tau_c$, alike the kinetic energy of the rattlers $K(t)$, with exponents compatible with $\psi_1$ and $\psi_2$. Similarly, the fluctuations of the elastic energy of the backbone, in the presence of a rescaling of the velocity of the rattlers by a factor $Q$, follow the same scaling as the overall kinetic energy, as in Fig. 2 (to be compared with Fig. 4). According to the fluctuation-dissipation theorem, fluctuations in the elastic energy can be related to the response of the system to an external perturbation. As a consequence, the energy fluctuations can be
FIG. 6: (color online) (Upper panel) Relaxation of the kinetic energy $K(\tau)$ of different replicas, following a rescaling of the rattlers velocity by a factor $Q$. (Lower panel) Data collapse according to Eq. 2.

FIG. 7: (Color online) (Upper panel) The standard deviation $\sigma_i(t)$, evaluated in logarithmic binned intervals, is plotted versus $\tau$ for different values of $Q$. We adopt the same symbols and colors of Fig. 5. In the inset the evolution of the potential energy for $Q = 1$. (Lower panel) The same data of $\sigma_i(t)$ rescaled according to Eq. (2) with the same value of $\alpha$ and $\tau_c$ used in Fig. 5.

IV. DISCUSSION

Investigating the dynamics of a granular system in the jammed state, we have shown that when the system jams due to the emergence of a network of contact forces able to sustain the applied stress, particle motion is not suppressed. Rather, the overall kinetic energy of the system becomes dominated by few rattler particles, that scatter inside their cages. Rattler-backbone collisions, surprisingly, stabilize the backbone. Thus, the larger the kinetic energy of the rattlers when the system jams, the smaller the time needed by the backbone to become rigid.

As a final remark we stress that there are strong similarities between the energy relaxation observed in our system and the one detected in the free cooling granular gas [32, 33]. Notwithstanding the striking difference in the granular density between the two systems, both exhibit a double power law decay with very similar values of the two exponents $\psi_1$ and $\psi_2$. Exploring if this similarity reflects some common mechanism beyond the relaxation of the two systems or it is just a coincidence is an interesting point to be addressed in future studies. Conversely, the relaxation of sheared frictionless granular systems occurring when the shear is turned off is qualitatively different, since it is found to follow an exponential decay [34].

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