Free-volume kinetic models of granular matter

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We show that the main dynamical features of granular media can be understood by means of simple models of fragile-glass-forming liquid [Kob and Andersen, Phys. Rev. E **48**, 4364 (1993)] provided that gravity alone is taken into account. In such lattice-gas models of cohesionless and frictionless particles, the compaction and segregation phenomena appear as purely nonequilibrium effects unrelated to the Boltzmann-Gibbs measure, which in this case is trivial. They provide a natural framework in which slow relaxation phenomena in granular and glassy systems can be explained in terms of a common microscopic mechanism given by a free-volume kinetic constraint.

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Vibrated powders are one of the most interesting examples of nonequilibrium systems where excluded-volume interactions are known to play a crucial role. Based on the free-volume notion, the analogy with glassy dynamics (and its limit) was recognized early [1]. Indeed, the static and dynamic properties of powders seem to be even more intriguing than those appearing in amorphous systems [2–6]. A natural question that arises is to what extent a powder can be considered as a glass [7,8].

In this paper, we show that compaction and segregation phenomena can be reproduced within a simple microscopic model of fragile-glass-forming liquid [9], provided that gravity alone is taken into account. The key ingredient of the model is a free-volume *kinetic* constraint involving only a selection of the possible configuration changes compatible with detailed balance and the Boltzmann-Gibbs distribution. Such kinetic constraints are so effective in describing slow relaxation phenomena that there is no need to invoke a specific energetic interaction or a particular geometry of particles. Consequently, the ground-state structure and the thermodynamics of the model turn out to be trivial. This is the most peculiar feature of this lattice-gas model as compared to the previously proposed ones (see, e.g., [10–14]). It follows that the nature of slow relaxation phenomena is not necessarily related to an equilibrium phase transition (as is the case of the critical slowing down); in particular, compaction and segregation phenomena are, at least in this case, purely dynamical effects unrelated to the Boltzmann-Gibbs measure. We find, therefore, that the subtle interplay of kinetic constraints and the gravity driving force can account for several experimental findings such as logarithmic compaction, vibration dependence of the asymptotic packing density, and segregation [15,16]. Such a phenomena appears below a well-defined vibration amplitude corresponding to the dynamical jamming transition of the model. Of course, the dynamics we consider is not intended to represent in a realistic way the microscopic granular dynamics but rather to provide an effective stochastic description, typically at the mesoscopic level.

The model we consider was introduced by Kob and Andersen as a lattice-gas model of fragile glass and used to test the predictions of the mode-coupling theory [9]. In its original version, the system consists of N particles on a simple-cubic lattice where there can be at most one particle per site. There is no cohesion energy among particles: the Hamiltonian is zero, $\mathcal{H}=0$. At each time step, a particle and one of its neighboring sites are chosen at random; the particle can move to the new site if it is empty and if the particle has less than ν nearest neighbors before and after it has moved. This kinetic rule is time-reversible and therefore the detailed balance is satisfied. At high density, the dynamics slows down because the reduced free volume makes it harder for a particle to meet the constraints. Above a certain threshold density, the particles are so interlocked that macroscopic structural rearrangements are no longer possible and the mobility steeply falls to zero. Such a mechanism is enough to provide the basic glassy phenomenology [9,17,18].

In the following, we consider the Kob-Andersen model in the presence of gravity. The system is described now by the Hamiltonian

$$\mathcal{H}=mg\sum_{i=1}^{N} h_i n_i , \tag{1}$$

where g is the gravity constant, $n_i=0,1$ are the occupation variables of the particles, and h_i is their height. We set the mass of particles throughout to 1, $m=1$. Particles are confined in a box closed at both ends and with a periodic boundary condition in the horizontal direction. We then assume that the random diffusive motion of ''grains'' produced by the mechanical vibrations on the box can be modeled by a thermal bath at temperature T: particles satisfying the kinetic constraints can move according to the Metropolis rule with probability $\min[1, x^{-\Delta h}]$, where $\Delta h=\pm 1$ is the vertical displacement in the attempted elementary move and $x=\exp(-g/T)$ represents the ''vibration.'' We set the constraint threshold at $\nu=5$. The system underlying geometry is that of a body-centered-cubic lattice. It gives the advantage of using a single parameter to describe the combined effect

of vibration and gravity. In this case, the Markov process generated by the kinetic rules is irreducible on the full configurations space provided that the box height is large enough: indeed it is always possible to find a path connecting any two configurations by letting, e.g., particles expand in the whole box. Therefore, the static properties of the model are those of a noninteracting lattice gas in a gravity field and they can be easily computed. We have investigated by extensive Monte Carlo (MC) simulation the dynamical behavior of this model for a system with $N=16\,000$ particles, height $16L$, and a transverse surface of $L^2/2$ sites, with $L=20$. The runs are carried out over 10^6 MC time sweeps (MCs) and the observables averaged typically over 20 realizations of dynamical evolution for each vibration amplitude x. The packing density is computed in the lower 25% of the system.

When particles are subject to gravity and no vibrations, $x=0$, the model has a single ground state with equilibrium packing density $\rho=1$. It could be attained, e.g., by letting the particles fall from the top of the box one at a time [19]. Therefore, we prepare the system in a fluffy initial state by placing the particles at random in the upper half of the box and letting them fall randomly, $x=0$, until they are not able to move anymore. We can assume that the mechanically stable state produced by this extensive statistical handling of particles represents a random loose-packed state. In this state, the average packing density turns out to be $\rho_{\mathrm{rlp}} \simeq 0.707$. Once the system is prepared in a fluffy configuration, the vibration with amplitude x is turned on. Instead of applying a sequence of taps, we used a continuous shaking procedure with the vibration kept constant, which is computationally more convenient and gives results qualitatively similar to the discontinuous tapping. In Fig. 1(a), we plot the packing density, $\rho(t)$, as a function of time for several values of x in the full range of weak and strong tapping. In spite of the relatively high value of ρ_{rlp} and the fact that kinetic constraints can be thought to mimic an effective short-range repulsion, the packing density slowly increases as time goes on and its asymptotic value is an increasing function of the vibration amplitude, even for quite high values of x, as in typical compaction experiments [15]. The slow increase of $\rho(t)$ is consistent, in the full range of weak and strong tapping, with a function of the form [15]

$$\rho(t)=\rho_\infty-\frac{\Delta\rho_\infty}{1+B\ln(1+t/\tau)} \tag{2}$$

[see Fig. 1(b)]. This inverse logarithmic law was first discovered in the experiments of the Chicago group [15], and is well supported by numerical simulations [12–14] and analytical approaches [20–22] essentially based on free-volume models. However, we find that in an intermediate range of vibration, a power-law fit also gives good results, while for stronger vibration, $x>0.3$, a modified logarithmic law works much better; a detailed discussion of these results will be presented elsewhere. We find that the fit parameters ρ_∞, B, and τ all depend on x. In particular, the asymptotic packing density, $\rho_\infty(x)$, is always smaller than 1 and it depends smoothly on x in agreement with the experimental results [15]. There is an optimal vibration amplitude, $x_{\max}\simeq 0.9$, at which ρ_∞ reaches a maximum; above $x_{\max}$, the asymptotic density become closer and closer to the equilibrium value

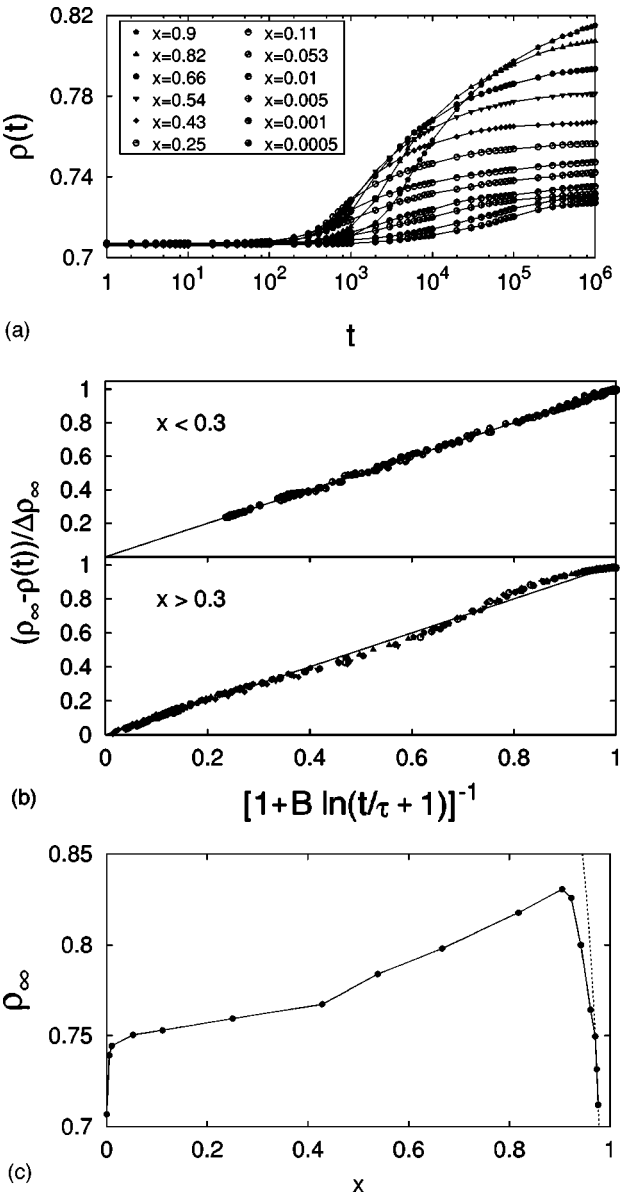

FIG. 1. Compaction experiment data: (a) packing density $\rho(t)$ computed in the lower 25% of the system vs time t for several values of the vibration amplitude x. The initial configuration is prepared in a random loose-packed state ($\rho_{\mathrm{rlp}}\simeq 0.707$); (b) logarithmic fit of compaction data in the weak ($x<0.3$) and strong ($x>0.3$) tapping regime. The fit parameters are all dependent on x. (c) Asymptotic value of packing density ρ_∞ vs x. The maximum occurs at $x_{\max}\simeq 0.9$ while the jamming transition point is at $x_g\simeq 0.96$. The dashed line represents the exact equilibrium packing density.

[see Fig. 1(c)]. The knowledge of thermodynamic properties allows us to find the point x_g above which the dynamical results coincide with the equilibrium ones. We find $x_g \simeq 0.96$ [see Fig. 1(c)]. This critical vibration amplitude defines the jamming transition of the model, which is the direct analog of the glass transition. Below x_g, the system is no longer able to equilibrate on the experimentally accessible time scales. This is essentially due to a *kinetic bottleneck*: at high packing density, the number of paths leading to the equilibrium configurations is much smaller than the one leading elsewhere. Therefore, even if the dynamics is in principle always able to reach equilibrium configurations, actu-

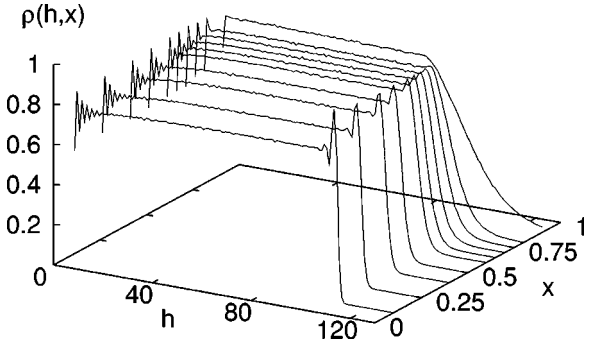

FIG. 2. Density profile $\rho(h,x)$ at time $t=2^{16}$ vs height h and vibration amplitude x. The bottom wall is located at $h=0$. Here the particle-wall interaction is ''attractive.''

ally for $x<x_g$ such configurations are not effectively accessible. We have checked that the usual MC procedure, obtained by removing the kinetic constraints, leads to the correct equilibrium configuration for any x. In this case, the equilibrium state is easily reached and the corresponding packing density $\rho_{\mathrm{eq}}(x)$ is a decreasing function of x. Paradoxically, $\rho_{\infty}(x)$ and $\rho_{\mathrm{eq}}(x)$ exhibit opposite monotony properties as long as $x<x_{\max}$.

We now turn to the behavior of the global density profile. In Fig. 2, we can observe that near the bottom wall the strong packing effects give rise to highly structured density profiles, with exponentially damped oscillations over a length scale that decreases with the vibration strength. This effect is interestingly similar to the layering phenomena appearing in simple fluids in confined geometry, which are usually interpreted in terms of the ''missing neighbors'' interaction of the particles near the wall [23]. In our case, the particle-wall interaction is purely kinetic: the ''particles'' building up the wall can affect or not the number of nearest-neighbor particles in the kinetic rule. We checked that in both cases the effect persists and results in a more or less dense bottom layer according to the ''attractive'' or ''repulsive'' nature of the kinetic particle-wall interaction. An experimental investigation of this point would be welcome. The exponential damping of these oscillations could explain why this fluid-like behavior is hardly observed in the experiments. A similar effect takes place near the top of the granular packing. However, due to the roughness of the free surface, the effect is less pronounced.

We finally consider the behavior of a mixture with different kinetic constraints. Indeed, size and mass segregation phenomena are another puzzling behavior exhibited by powders, and several distinct mechanisms have been proposed [16,24–26]. Our main concern here is to show that, in their simplest form, segregation phenomena also appear in the present model. To keep things as simple as possible, we consider only the case of a binary mixture with particles of identical mass. The only difference between the two components is purely kinetic: one type of particle is constrained while the other one is not; the latter particles can, however, block the former ones. The Hamiltonian of the system is given by Eq. (1), and the microscopic reversibility is still satisfied. In Fig. 3, we plot the time evolution of the density profile of a binary mixture starting from a random homogeneous distribution of particles. Although the packing fraction of both components increases, the system undergoes, at the same time, a spontaneous unmixing with the constrained particles segregating at the top of the mixture (see Fig. 3). This turns out to be the case even when the mass of constrained particles is bigger than the unconstrained ones, at least in a certain range of the mass ratio of the two components. Such an effect can be simply explained in terms of the different mobilities: during the shaking process, the unconstrained ''small'' particles easily fill the gap beneath the constrained ''large'' particles whenever they open up; this decreases the probability of the slower constrained particles falling down. A similar percolation or sifting mechanism was found in Ref. [27]. In our case, it is clearly not related to an equilibrium phase transition, since the Hamiltonian is ''blind'' to the constraints.

To summarize, we have investigated some aspects of granular dynamics in a three-dimensional gravity-driven lattice-gas model. The key ingredient of the model is a free-volume constraint implemented in a purely kinetic way [9]. Below a critical value of vibration, the system undergoes a purely dynamical jamming transition. For weak vibrations, the packing density logarithmically increases towards an asymptotic value that depends on the vibration amplitude, in agreement with experiments [15]. Near the bottom wall and the free surface of the granular cluster, the strong packing effects induce highly structured density profiles; this phenomenon could be closely related to the one appearing in confined liquids. When a mixture of particles with different constraints is considered, a vibration-induced phase separation appears in the system. We emphasize that the results mentioned above are obtained in a model with trivial thermodynamics without introducing any form of quenched randomness either in the energetic interaction or in the shape of particles. Therefore, all interesting effects have a purely dynamical nature and manifest themselves as a departure from the Boltzmann-Gibbs equilibrium measure. It would be interesting to derive these nonequilibrium features in terms of the Edwards measure [28].

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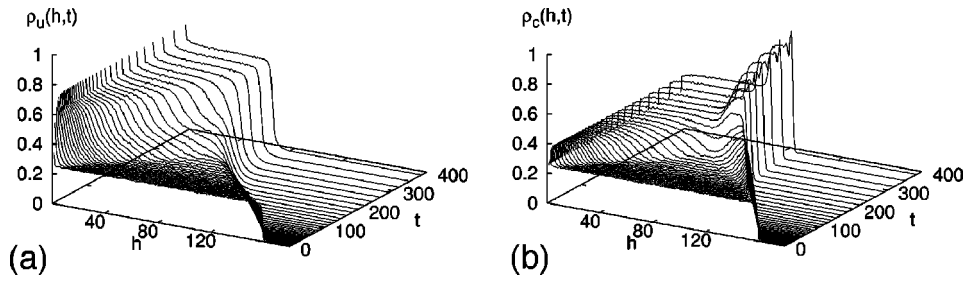

FIG. 3. Density profile of a 1:1 binary mixture vs height h and time t. (a): unconstrained particles; (b): constrained particles. The vibration amplitude is $x=0.1$. The system was prepared in a random homogeneous initial state.

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