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Effective temperature of an aging powder

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The aging dynamics and the fluctuation-dissipation relation between the spontaneous diffusion induced by a random noise and the drift motion induced by a small stirring force are numerically investigated in a 3D schematic model of compacting powder: a gravity-driven lattice-gas with purely kinetic constraints. The compaction dynamics is characterized by a super-aging behavior and, in analogy with glasses, exhibits a purely dynamical time-scale-dependent effective temperature. A simple experiment to measure this quantity is suggested.

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INTRODUCTION

Slow relaxation phenomena are ubiquitous in nature. When one deals with glassy dynamics the challenge is the identification of the relevant degrees of freedom which makes a thermodynamic description still possible. In the attempt to provide a unifying framework to the behavior of aging and nonrelaxational systems, a microscopic definition of effective temperature was introduced through a generalized fluctuation-dissipation relation [1]. This quantity turns out to coincide, at least in mean-field glasses, with the Edwards' compactivity [2–5], previously introduced in a granular matter context [6,7]. For a class of finite-dimensional and zero-gravity compacting systems, recent numerical results have come to support this correspondence [8]. However, in contrast to the case of strong [9], or moderately strong [10] vibration regime, the absence of a temperaturelike quantity in slowly driven compacting systems under gravity is a rather problematic issue [11–13]. In this Rapid Communication we investigate the nature of the aging dynamics and the effective temperature in a simple three-dimensional (3D) lattice-gas model of powder [14]. We show that the nonequilibrium dynamics is characterized by a three-step relaxation mechanism and ''super-aging'' in the mean-square displacement. We then find that during the compaction the response to a random perturbation is positive and observe a violation of the fluctuation-dissipation relation similar to glasses. Such features show that it is possible to describe the gravity driven compaction dynamics in terms of a purely dynamical time-scale-dependent effective temperature.

MODEL

The model we consider was introduced in Ref. [14] as a simple generalization of the Kob-Andersen model [15]. The system consists of N particles on a body centered cubic lattice where there can be at most one particle per site. There is no cohesion energy among particles and the Hamiltonian is simply

$$\mathcal{H}_0 = mg\sum_{i=1}^{N} h_i , \tag{1}$$

where g is the gravity constant, h_i is the height of the particle i, and m its mass. At each time step a particle can move with probability p to a neighboring empty site if the particle has less than ν nearest neighbors before and after it has moved. Here $p=\min[1,x^{-\Delta h}]$, where $\Delta h=\pm 1$ is the vertical displacement in the attempted elementary move and $x=\exp(-mg/T)$ represents the ''vibration.'' The kinetic rule is time-reversible and hence, the detailed balance is satisfied. We therefore assume that statistical properties of the mechanical vibrations on the box can be described, after a suitable coarse-graining, as a thermal bath at temperature T. In the regime of quasistatic flow this assumption, which neglects the complicated effects like friction and dissipation between grains, is a reasonable starting point [6]. We set throughout the mass $m=1$ and the threshold $\nu=5$. Particles are confined in a box closed at both ends and with periodic boundary condition in the horizontal direction. We consider a system of height $16L$ and transverse surface L^2 with $L=20$, and number of particles $N=16\,000$ (corresponding to a global density of 0.25). As shown in Ref. [14], the interplay of kinetic constraints and gravity are enough to reproduce the basic aspect of weakly vibrated powderlike compaction and segregation phenomena, and vibration-dependent asymptotic packing density. In the following we consider the nonequilibrium features as they show up in the two-time correlation and response function.

AGING DYNAMICS

Slow relaxation in weakly vibrated powder is closely related to the reduction of the free volume available to the particle motion; hence, age-dependent properties are expected [16–18]. The aging dynamics in simple models of granular matter has been recently studied by several authors [12,13,19,20]. For our purposes it can be easily characterized in terms of the ''mean-square displacement'' between two configurations at time t_w and $t>t_w$,

$$B(t,t_w)=\frac{1}{N}\sum_{i=1}^{N}\langle[h_i(t)-h_i(t_w)]^2\rangle, \tag{2}$$

where the angular brackets denote the average over the random noise. The system is initially prepared in a random loose packed state, which in this model corresponds to a

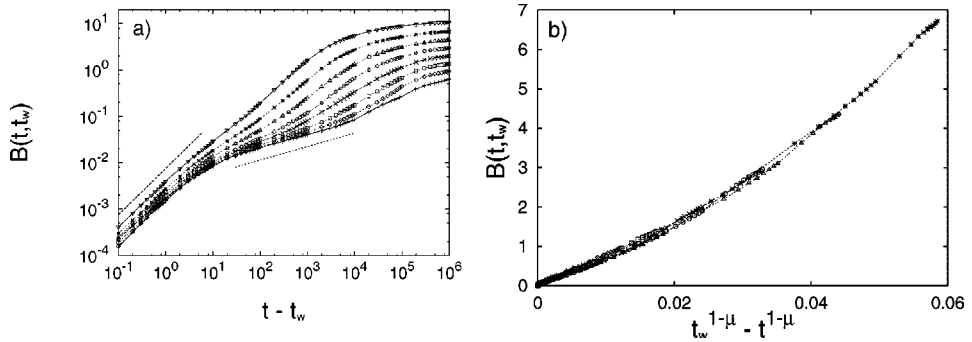

FIG. 1. (a) Mean-square displacement $B(t,t_w)$ vs $t-t_w$ measured from a random loose packed initial state ($\rho_{\rm rlp}\simeq 0.707$). The vibration amplitude is $x=0.2$, and waiting times are $t_w=2^k$ with $k=10,\ldots,17$ (from the top to the bottom). The dashed line represents the short-time normal diffusion regime. (b) The same data plotted vs the scaling variable $t_w^{1-\mu}-t^{1-\mu}$. The super-aging exponent is $\mu\simeq 1.41$ for $x=0.2$.

packing density $\rho_{\rm rlp}\simeq 0.707$ [14], and then the vibration is turned on. The plot of $B(t,t_w)$, see Fig. 1(a), clearly shows the well known aging effect. The system does not reach any equilibrium state on the observation time-scale, but rather persists in a nonstationary regime: the particle displacements become slower and slower as the age of the system increases. Interestingly, Fig. 1(a) shows a three step relaxation mechanism: a short-time normal diffusion; an intermediate subdiffusive regime which is tempting to associate to the ''cage rearrangement;'' and finally, a relatively faster but still subdiffusive regime which can be figured out as a ''cage-diffusion.'' Inspired by recent analytic results on a related anomalous diffusion model [21], we use a scaling function representing a super-aging behavior. In Fig. 1(b) the mean-square displacement data are plotted versus the variable $t_w^{1-\mu}-t^{1-\mu}$. We find that the value $\mu\simeq 1.41$ gives a quite good data collapse for vibration $x=0.2$ [Fig. 1(b)]. The exponent μ appears to increase with the vibration, at least on the accessible time-scale of our simulations. We obtain, for instance, $\mu\simeq 1.28$ for $x=0.05$ and $\mu\simeq 1.48$ for $x=0.4$. According to the theory presented in Ref. [21] the exponent is universal and its value is $\mu\simeq 1.48$. We believe that the discrepancy observed at small x is due to the fact that the system is still far from the asymptotic high packing density regime where the predictions of Ref. [21] apply. In the super-aging regime, the characteristic relaxation time of the system grows faster than its age, a rather unusual feature as compared to glassy polymers or random magnets [18].

EFFECTIVE TEMPERATURE

The possibility of a thermodynamic description of slow relaxing systems is apparently ruled out by the breakdown of time-translation invariance, i.e., the presence of aging phenomena. In granular materials further complications may arise from the presence of spatial inhomogeneities induced by the boundary conditions and the gravity direction. In analogy with glassy systems we show, however, that the violation of the fluctuation-dissipation relation is not arbitrary. It is such that the degrees of freedom associated with the slow motion can be considered as equilibrated at an effective temperature (vibration) higher than the one imposed by the external bath (forcing). In order to see this we need to compute the dynamical response function. We apply to the system a small random stirring force at time t_w,

$$\mathcal{H}_\epsilon=\mathcal{H}_0+\epsilon\sum_{i=1}^{N} f_i h_i, \tag{3}$$

where $f_i=\pm 1$ independently for each particle. The linear regime is probed for small enough values of the perturbation ϵ. The integrated response function conjugated to Eq. (2) is the ''staggered displacement''

$$\kappa(t,t_w)=\frac{1}{N}\sum_{i=1}^{N}\langle\overline{f_i[h_i(t)-h_i(t_w)]}\rangle. \tag{4}$$

where the overline denotes the average over the random stirring force. At thermal equilibrium κ and B are time-translation invariant and the Einstein relation holds,

$$\kappa(t-t_w)=\frac{\epsilon}{2T}B(t-t_w). \tag{5}$$

It has been suggested that a simple generalization of the previous relation in the aging regime provides, in a suitable long-time limit, a reliable definition of effective temperature [1],

$$T_{\rm eff}(t,t_w)=\frac{\epsilon}{2}\frac{B(t,t_w)}{\kappa(t,t_w)}. \tag{6}$$

In a class of solvable mean-field models of glasses [18], $T_{\rm eff}(t,t_w)$ has the following properties. When $t-t_w\sim O(t_w)$, $T_{\rm eff}(t,t_w)=T$; while for $t/t_w\gg O(1)$, $T_{\rm eff}(t,t_w)$ is a constant or slowly waiting-time-dependent quantity higher than the bath temperature T. In recent experiments, effective temperature has been measured in glycerol [22] and laponite [23].

In order to measure the effective temperature the system is first prepared in a random loose packed state. Then it compacts for a time t_w under a given vibration, x. At t_w the random perturbation is applied, and the staggered displacement between configurations at times t_w and t is measured. Following this method we find a positive monotonic re-

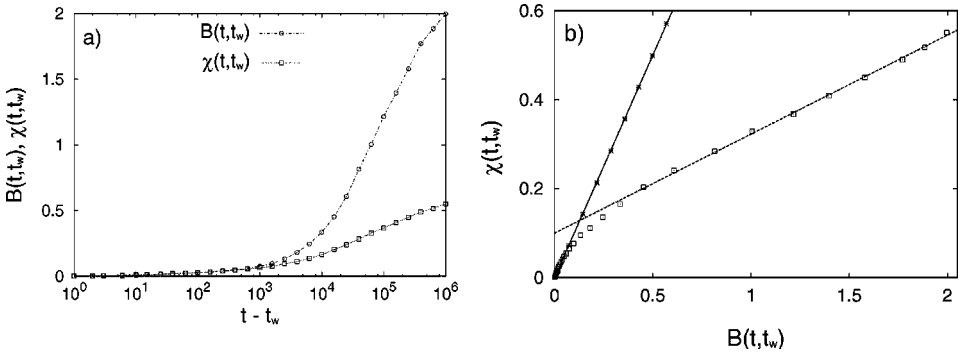

FIG. 2. Measuring the nonequilibrium fluctuation dissipation relation in a compaction experiment. The system is prepared in a random loose packed state, $\rho_{\rm rlp} \simeq 0.707$, and then shaken with a vibration $x=0.2$. The system compacts for a waiting time $t_w = 2^{14}$ after which a small stirring force is turned on. (a) Comparison of the mean-square displacement $B(t,t_w)$ and the conjugated response function $\chi(t,t_w) = 2T\,\kappa(t,t_w)/\epsilon$ vs $t-t_w$. (b) Parametric plot of $B(t,t_w)$ vs $\chi(t,t_w)$. The slope of the dashed line is $\simeq 0.22$. The solid line is the equilibrium fluctuation-dissipation theorem, which is correctly recovered in the zero-gravity limit, when particles diffuse in the whole box and the system reaches a low-density regime.

sponse function. At small time separation the integrated response and correlation are equal, while at later time they depart from each other, with the response increasing slower than the corresponding correlation [see Fig. 2(a)]. The nature of the violation of the fluctuation-dissipation relation is best represented in the parametric plot of $\kappa(t,t_w)$ versus $B(t,t_w)$. In Fig. 2(b) is shown such a plot for a waiting time $t_w = 2^{14}$ Monte Carlo sweeps and vibration $x=0.2$. In close analogy with glassy systems we observe two ''quasiequilibrium'' regimes. At short time the usual equilibrium fluctuation-dissipation relation holds and $T_{\rm eff}(t,t_w)=T$. At later time a strong violation of the fluctuation-dissipation relation is observed. In this regime the numerical data can be fitted with an excellent approximation by a straight line. This means that the slope of the parametric plot does not depend on the observation time and therefore the effective temperature may only depend on t_w. A closer inspection of Figs. 1 and 2 reveals that the crossover between the two quasiequilibrium regimes takes place over a time scale corresponding to the ''cage-rearrangement'' motion. The picture outlined above holds in the whole range of weak vibrations $0.05 \leqslant x \leqslant 0.4$ and waiting times $t_w \leqslant 10^5$ that we have explored. In particular, we find that the effective temperature decreases with the external vibration (bath temperature) and slowly with the waiting time t_w.

Finally, to clarify some problems raised in Ref. [11], and discussed in detail in Ref. [12], we have also studied the response function to a *uniform*, either positive or negative, force field. In both cases we find a nonmonotonic response function with a negative component. In particular, when kinetic constraints are removed and the system is at equilibrium, the thermal bath temperature is not recovered with this method. This shows the importance of using stochastic perturbations to define the temperature from the fluctuation-dissipation relation.

CONCLUSION

The notion of effective temperature has been often invoked as the first step towards the formulation of a nonequilibrium statistical mechanics for systems as different as vibrated powders [6,7], turbulent fluids [24], and structural glasses [1,5]. We have shown in this paper that a purely dynamical time-scale-dependent effective temperature appears during the compaction dynamics of 3D constrained lattice-gas models of aging powder. Mean-field glassy models suggest that such a feature is robust with respect to nonrelaxational perturbations [1] and time-dependent driving forces [25]. Preliminary results confirm this expectation in more realistic, Hertz contact mechanics based models [26].

It is worth noting that the perturbed Hamiltonian (3) describes a particle system with a random distribution of mass with average m and standard deviation proportional to ϵ. Hence, the measure of the effective temperature presented here could be experimentally carried out in a suitably prepared sample of glass beads, provided that ϵ is small enough to probe the linear response regime, and that mass-segregation effects are negligible. With the particle tracking experimental facilities (such as, for instance, PEPT [27]), this measure might not be out of reach.

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