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Definition of temperature in dense granular media

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In this paper we report the measurement of a pseudotemperature for compacting granular media on the basis of the fluctuation-dissipation relations in the aging dynamics of a model system. From the violation of the fluctuation-dissipation theorem emerges an effective temperature (a dynamical temperature T_{dyn}) whose value depends on the particle density. We compare the results for T_{dyn} at several densities with the values of Edwards' compactivity at the corresponding densities [S. F. Edwards, in *Granular Matter: An Interdisciplinary Approach*, edited by A. Mehta (Springer-Verlag, New York, 1994) and references therein]. It turns out that the dynamical temperature and Edwards' compactivity coincide on a large range of densities, opening in this way the door to experimental checks as well as theoretical constructions.

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The study of compact granular matter through statistical physics tools is a subject of sustained interest [1]. Granular media enter only partially into the framework of equilibrium statistical mechanics and their dynamics constitutes a very complex problem of nonequilibrium which poses novel questions and challenges to theorists and experimentalists. The very possibility of constructing a coherent statistical mechanics for these systems is still a matter of debate, although everybody agrees that such an approach, if possible, would allow for a much deeper and global understanding of the problem.

One of the main obstacles in this direction is the nonthermal character of these systems: thermal energy is so negligibly small with respect to other energy contributions (e.g., potential energy) that for all practical purposes these systems live virtually at zero temperature. One of the most important consequences is that, unless perturbed in some way (e.g., driving energy into the system), a granular system cannot explore spontaneously its phase space but remains trapped in one of the numerous metastable configurations. Understanding the structure of the phase space which is left invariant by the dynamics is then crucial for the construction of a thermodynamical description of these nonthermal systems.

A very ambitious approach, in this direction, has been put forward by Edwards and Mehta *et al.* [2,3], by proposing an equivalent of the microcanonical ensemble: macroscopic quantities in a jammed situation should be obtained by a flat average over all *blocked configurations* (i.e., in which every grain is unable to move) of given volume, energy, etc. The strong assumption here is that all blocked configurations are treated as equivalent and have the same weight in the measure. This approach, based on the idea of describing granular material with *a small number of parameters*, leads to the introduction of an entropy S_{edw}, given by the logarithm of the number of blocked configurations of given volume, energy, etc., and its corresponding density $s_{edw} \equiv S_{edw}/N$. Associated with this entropy are the state variables such as "compactivity," $X_{edw}^{-1} = \partial S_{edw}/\partial V(V)$ and, "temperature" $T_{edw}^{-1} = \partial S_{edw}/\partial E(E)$.

Very recently, important progress in this direction has been reported in various contexts: a tool to systematically construct Edwards' measure, defined as the set of blocked configurations of a given model, was proposed in [4,5]; it was used to show that the values of various observables in the aging dynamics of the Kob-Andersen model (a kinetically constrained lattice-gas model) were correctly predicted by Edwards' measure. Moreover, the validity and relevance of Edwards' measure have been demonstrated for one-dimensional phenomenological models [6], for spin models with "tapping" dynamics [7], and for sheared hard spheres [8].

In this paper, we focus on the possibility of defining a pseudotemperature for granular media, in the framework of the aging dynamics of a model system [9]. From the violation of the fluctuation-dissipation theorem (i.e., from a *dynamical* measure) emerges an effective temperature (from here on indicated as dynamical temperature T_{dyn}) whose value depends on the particle density. We show that the dynamical temperature coincides on a large range of densities with the *statically* obtained Edwards' compactivity. This allows for a thermodynamical interpretation of T_{dyn}, and opens the door to experimental checks as well as theoretical constructions.

It is interesting to mention recent approaches that are complementary to ours. On the one hand, in the context of aging supercooled liquids, the inherent structure strategy does not address the question of a determination of a static distribution, but promising results show that this measure, if it exists, is insensitive to the details of the thermal history [10]. The link between this strategy and Edwards' measure has been discussed in [5,11]. On the other hand, recent works on the possibility of a dynamical definition of temperature have focused on sheared, stationary systems [12,13]. These studies are clearly complementary to the present one, which addresses the problem of the relation between the value of T_{dyn} and a static measure, in aging (nonstationary) systems.

The model we consider is a version of the "Tetris" model [9], which has been shown to reproduce several features of granular media, such as aging [16,17], memory [18], self structuring [19], etc. In the framework of this model, some of us have already provided evidence of the validity of Edwards' measure [5].

We focus in particular on a case of a homogeneous system with no preferred direction in order to avoid any kind of instability or large-scale structure formation [19]. The case with gravity which imposes a preferential direction will be discussed elsewhere [15] and we shall limit ourselves here to summarizing the main results. In the version of the model that we use, "T"-shaped particles diffuse on a square lattice, with the only constraint being that no superposition is allowed: for two nearest-neighbor particles, the sum of the arms oriented along the bond connecting the two particles has to be smaller than the bond length (for each particle, the three arms of the "T" have length $\frac{3}{4}d$, where d sets the bond size of the square lattice). The maximum density allowed is then $\rho_{max}=2/3$. This model represents a clear example of a nonthermal system. The Hamiltonian is zero and the temperature itself is therefore irrelevant at equilibrium, only its ratio with an imposed chemical potential being important.

The out-of-equilibrium compaction dynamics without gravity is implemented as follows: starting from an empty lattice, particles are randomly deposited, without diffusion and without violation of the geometrical constraints. This random sequential absorption process yields a reproducible initial density of $\rho\approx 0.547$. Alternating diffusions and additions of particles are then attempted, making it possible to increase the density of the system, which remains homogeneous in the process. In order to overcome the problem related to the simulation of slow processes and obtain a reasonable number of different realizations to produce clean data, we have devised a fast algorithm (in the spirit of the Bortz-Kalos-Lebowitz algorithm [20]) where the essential ingredient is the updating of a list of mobile particles (whose number is n_{mob}), i.e., of particles that are not blocked by the geometrical constraints. At each time step a mobile particle is selected, and moved in the direction chosen only if no violation of the constraints occurs. If the attempt has been successful, the list of mobile particles is then updated, performing a *local* control of the grains' mobility. This procedure therefore introduces a temporal bias in the evolution of the system, which has to be taken into account by incrementing the time of an amount $\Delta t=1/n_{mob}$, after each guided elementary step. This algorithm becomes very efficient as the density of the system increases, since the number of mobile particles decreases drastically.

We have simulated lattices of linear size $L=50$, 100, and 200, in order to ensure that finite-size effects were irrelevant. We have chosen periodic boundary conditions on the lattice, having verified that other types of boundary conditions (e.g., closed ones) gave the same results.

During the compaction, we monitor the following quantities: the density of particles $\rho(t)$ and the density of mobile particles $\rho_{mob}(t)$. Moreover, in order to establish the fluctuation-dissipation relations, we measure the mean-square displacement $B(t+t_w,t_w)$ and the integrated response function $\chi(t+t_w,t_w)$. The mean-square displacement is defined as

$$B(t+t_w,t_w)=\frac{1}{N}\sum_{i=0}^{N}\sum_{r=x,y}\langle[r_i(t+t_w,t_w)-r_i(t_w)]^2\rangle,$$

where N is the number of particles present in the system at time t_w, r_i is the coordinate (x or y) of the ith particle, and the brackets $\langle\ \rangle$ indicate the average over several realizations.

In order to measure the integrated response function $\chi(t+t_w,t_w)$, we make a copy of the system at time t_w and apply to it a small random perturbation, varying the diffusion probability of each particle from $p=\frac{1}{4}$ to $p^{\epsilon}=\frac{1}{4}+f_i^r\times\epsilon$, where $f_i^r=\pm 1$ is a random variable associated to each grain independently for each possible direction ($r=x,y$), and ϵ represents the perturbation strength. For a constant field we obtain (see also [4,5,15])

$$\chi(t+t_w,t_w)=\frac{1}{2\epsilon N}\sum_{i=1}^{N}\sum_{r=x,y}\langle f_i^r\Delta r_i(t+t_w)\rangle, \tag{1}$$

where $\Delta r_i(t+t_w)=r_i^{repl}(t+t_w)-r_i(t+t_w)$ is the difference between the displacements that take place in the two systems evolving with the same succession of random numbers. In this communication, we present the results obtained with a perturbation strength $\epsilon=0.005$, having checked that for $0.002<\epsilon<0.01$, nonlinear effects are absent.

If the system were in equilibrium we would expect B and χ to be linearly related by

$$2\chi(t+t_w,t_w)=\frac{X}{T_d^{eq}}B(t+t_w,t_w), \tag{2}$$

where X is the so-called fluctuation-dissipation ratio (FDR) which is unitary in equilibrium. Any deviations from this linear law signals a violation of the fluctuation-dissipation theorem (FDT). Nevertheless it has been shown, first in mean-field models [21], then in various simulations [22,23] how in several aging systems violations from Eq. (2) reduce to the occurrence of two regimes: a quasiequilibrium regime with $X=1$ (and time-translation invariance) for "short-" time separations ($t\ll t_w$), and the aging regime with $X\leqslant 1$ for large time separations. This second slope is typically referred to as a dynamical temperature $T_{dyn}\geqslant T_d^{eq}$ such that $X=T_d^{eq}/T_{dyn}$ [24].

In our case, as the density increases, an aging behavior is obtained: the system falls out of equilibrium and $\rho_{mob}(t)$ gets smaller than the corresponding value at equilibrium [5]. Accordingly, violations of Eq. (2) are expected.

If the compaction process is stopped at a certain time t_w, the system relaxes toward equilibrium and one obtains a time-translation-invariant behavior for χ and B; this is the so-called regime of interrupted aging which features an increase of ρ_{mob} to its equilibrium value and a single linear relation for the χ vs B parametric plot. These measures there-

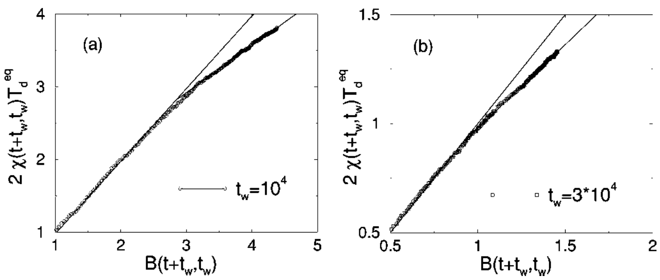

FIG. 1. Einstein relation in the Tetris model: plot of the mobility $2\chi(t_w+t,t_w)T_d^{eq}$ vs the mean-square displacement $B(t_w+t,t_w)$, for $t_w^1=10^4$ and $t_w^2=3\times10^4$. The slope 1 of the full straight line corresponds to the equilibrium case, obtained for the dynamics at constant density (interrupted aging).

fore give us the value of the equilibrium fluctuation-dissipation ratio T_d^{eq}, which actually does not depend on the density reached at t_w.

If, on the other hand, the compaction process is not stopped, the system features an aging behavior and the χ vs B parametric plots, displayed in Fig. 1, show two different linear behaviors: after a first quasiequilibrium regime in which the plot has slope T_d^{eq}, a violation of FDT is observed, with the existence of a dynamical temperature T_{dyn} which depends on t_w and therefore on the density. We denote as $X_{dyn}=T_d^{eq}/T_{dyn}$ the ratio between the equilibrium and non-equilibrium slopes, and measure $X_{dyn}^1=0.646\pm0.002$, $X_{dyn}^2=0.767\pm0.005$, $X_{dyn}^3=0.784\pm0.005$ at $t_w^1=10^4$, $t_w^2=3\times10^4$, and $t_w^3=5\times10^4$. We are now able to compare the values of the dynamical measures with the outcome of Edwards' measure. The construction of the equilibrium and Edwards' measures has been described in [5]. In particular, an efficient sampling of the blocked configurations, and therefore Edwards' measure, is obtained by the use of an auxiliary model whose energy is defined to be the number of mobile particles: the introduction of an auxiliary temperature and an annealing procedure then yields configurations with no mobile particles. Having computed equilibrium and Edwards' entropies as a function of density, as in [4,5], we measure the ratio of the slopes (that we denote as Edwards' ratio)

$$X_{Edw}=\frac{ds_{Edw}(\rho)}{d\rho}/\frac{ds_{equil}(\rho)}{d\rho}, \tag{3}$$

which is plotted in Fig. 2. This ratio approaches 1 as $\rho\to2/3$, since at the maximum density all configurations become blocked and therefore equilibrium and Edwards' measures become equivalent.

The values of the dynamical fluctuation-dissipation ratio are also reported in the same figure (with no error bars since they are too small) and yield the following densities: $\rho_1\approx0.596$ for $t_w^1=10^4$, $\rho_2\approx0.603$ for $t_w^2=3.10^4$, $\rho_3\approx0.605$ for $t_w^3=10^5$. On the other hand, the evolution of the density of the system during the measurements is reported in Fig. 3.

Since the measurements are performed *during* the compaction, the density is evolving, going from $\rho(t_w)$ to $\rho(t_w+t_{max})$. In each case, we obtain that indeed ρ_i

TABLE I. Fluctuation-dissipation ratio (FDR) as obtained from numerical data fits with the corresponding densities obtained from Fig. 2. The last column reports the density intervals explored during the compaction dynamics (starting from the times where deviations from equilibrium become evident) for $t_w=10^4$, 3×10^4, 5×10^4.

	FDR	density	density interval
$t_w=10^4$	0.646	0.596	[0.584,0.597]
$t_w=3\times10^4$	0.767	0.603	[0.599,0.605]
$t_w=5\times10^4$	0.784	0.605	[0.603,0.606]

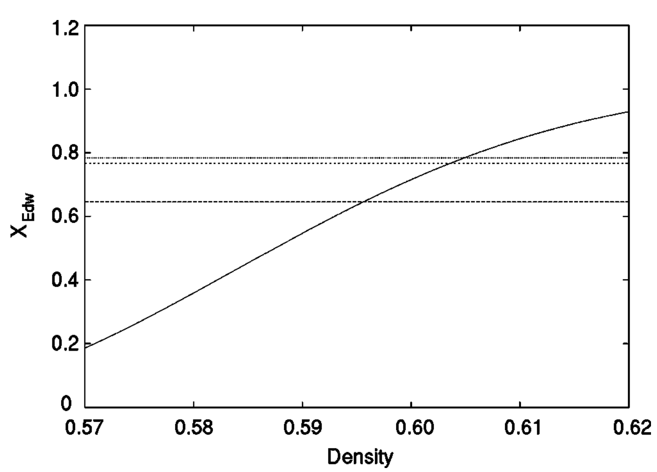

FIG. 2. Edwards' ratio X_{Edw} as a function of density. The horizontal lines correspond to the dynamical ratios X_{dyn}. measured at $t_w=10^4$, 3×10^4, 5×10^4 and determine the values $\rho_1\approx0.596$, $\rho_2\approx0.603$, $\rho_3\approx0.605$, to be used in the comparison with the results reported in Fig. 2.

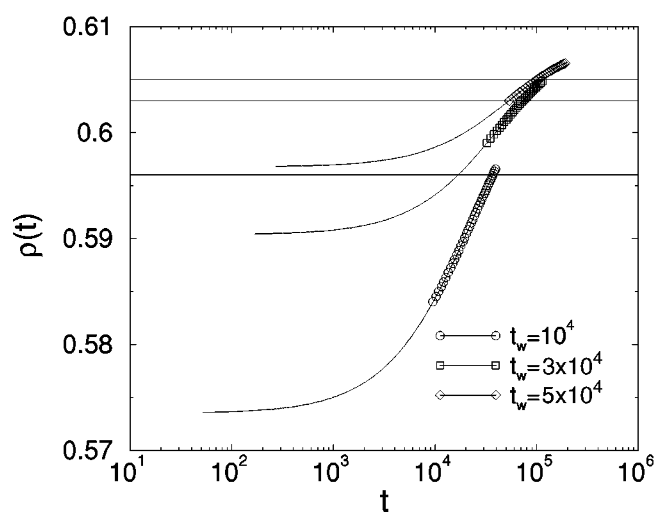

FIG. 3. Evolution of the density during the measurements of χ and B, for $t_w=10^4$, 3×10^4, 10^5. The evolution during the quasiequilibrium part is plotted with lines, and during the violation of FDT with symbols. The horizontal lines correspond to the densities ρ_1, ρ_2, ρ_3 from Fig. 3.

$\in[\rho(t_w^i),\rho(t_w^i+t_{max})]$, where we have denoted with ρ_i the densities obtained from Fig. 2 for different values of $t_w(i=1,2,3)$. More precisely, ρ_i is very close to $\rho(t_w^i+t_{max})$. This is to be expected, since the measure of the FDT violation is made for times much larger than t_w^i and, since the compaction is logarithmic, the system actually spends more time at densities close to $\rho(t_w^i+t_{max})$ than to $\rho(t_w^i)$.

The validation of Edwards' hypothesis in various model systems has made important steps forward recently; here we have focused, for a model with only geometrical constraints, on the definition of a dynamical temperature and its link with Edwards' measure. While the density increases, the measured dynamical temperature decreases, following closely the ratio between the equilibrium and Edwards' entropies, the latter being obtained through a flat sampling of blocked configurations. While Edwards' proposal is supposed to be only asymptotically valid, i.e., when one-time quantities are almost stationary, our study clearly shows that it actually yields good results even in a preasymptotic regime, when the density is still evolving a lot.

In this paper, the idealized case of a homogeneously compacting system has been investigated. The limitations of the validity of Edwards' measure are still to be investigated. In particular, we will investigate the case of a compacting system under gravity, i.e., with a preferred direction, in [15].

Another crucial point concerns the fact that the dynamically defined effective temperature could *a priori* depend on the observables used for the measure of the violation of the FDT. Its interpretation as a temperature in a thermodynamical sense would then be questionable. While the effective temperature is known to be observable independent of mean-field models, this question has been addressed only recently in realistic models: two recent studies on sheared (stationary) thermal [12] and athermal [13] systems show the consistency of various definitions [14]. Our results complement these studies by allowing us to relate the value of T_{dyn} to a static measure. Moreover, the observable independence character of T_{dyn} in our case will be checked in [15], by considering systems consisting of two types of particles. In this respect, the presence of a preferred direction could imply limitations; for sheared, stationary systems, a preferential direction exists, but only measures along the other directions have been performed [8,25,12,13].

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[1] *Physics of Dry Granular Media*, edited by H. J. Herrmann and S. Luding (Kluwer Academic, Dordrecht, The Netherlands, 1998), p. 553–583.
[2] S. F. Edwards, in *Granular Matter: An Interdisciplinary Approach*, edited by A. Mehta (Springer-Verlag, New York, 1994), and references therein.
[3] A. Mehta, R. J. Needs, and S. Dattagupta, J. Stat. Phys. **68**, 1131 (1992).
[4] A. Barrat, J. Kurchan, V. Loreto, and M. Sellitto, Phys. Rev. Lett. **85**, 5034 (2000).
[5] A. Barrat, J. Kurchan, V. Loreto, and M. Sellitto, Phys. Rev. E **63**, 051301 (2001).
[6] J. J. Brey, A. Prados, and B. Sanchez-Rey, Phys. Rev. E **60**, 5685 (1999); Physica A **A275**, 310 (2000).
[7] D. S. Dean and A. Lefévre, Adv. Complex Syst. **4**, 333 (2001), and references therein.
[8] H. Makse and J. Kurchan, e-print cond-mat/0107163.
[9] E. Caglioti, V. Loreto, H. J. Herrmann, and M. Nicodemi, Phys. Rev. Lett. **79**, 1575 (1997).
[10] W. Kob, F. Sciortino, and P. Tartaglia, Europhys. Lett. **49**, 590 (2000).
[11] A. Fierro, M. Nicodemi, and A. Coniglio, e-print cond-mat/0107134.
[12] L. Berthier and J. L. Barrat, e-print cond-mat/0110257.
[13] I. K. Ono, C. S. O'Hern, S. A. Langer, A. J. Liu, and S. R. Nagel, e-print cond-mat/0110276.
[14] The models considered in [12,13] are sheared, and therefore present a preferred direction. However, the observables under investigation concern only the other directions.
[15] V. Colizza, V. Loreto, and A. Barrat (unpublished).
[16] M. Nicodemi and A. Coniglio, Phys. Rev. Lett. **82**, 916 (1999).
[17] A. Barrat and V. Loreto, J. Phys. A **33**, 4401 (2000).
[18] A. Barrat and V. Loreto, Europhys. Lett. **53**, 297 (2001).
[19] S. Krishnamurthy, V. Loreto, H. J. Herrmann, S. S. Manna, and S. Roux, Phys. Rev. Lett. **83**, 304 (1999); S. Krishnamurthy, V. Loreto, and S. Roux, *ibid.* **84**, 1039 (2000).
[20] A. Bortz, M. H. Kalos, and J. L. Lebowitz, J. Chem. Phys. **17**, 10 (1975).
[21] L. F. Cugliandolo, J. Kurchan, Phys. Rev. Lett. **71**, 173 (1993); J. Phys. A **27**, 5749 (1994).
[22] G. Parisi, Phys. Rev. Lett. **79**, 3660 (1997).
[23] W. Kob and J. L. Barrat, Europhys. Lett. **46**, 637 (1999).
[24] L. F. Cugliandolo, J. Kurchan, and L. Peliti, Phys. Rev. E **55**, 3898 (1997).
[25] J.-L. Barrat and L. Berthier, Phys. Rev. E **63**, 012503 (2001).