On the definition of temperature in dense granular media

Vittoria Colizza\(^1\), Alain Barrat\(^2\) and Vittorio Loreto\(^1\)

\(^1\) Università degli Studi di Roma “La Sapienza”, Dipartimento di Fisica, P.le A. Moro 5, 00185 Rome, Italy and INFM, Unità di Roma 1

\(^2\) Laboratoire de Physique Théorique Unité Mixte de Recherche UMR 8627, Bâtiment 210, Université de Paris-Sud, 91405 Orsay Cedex, France

(Dated: November 17, 2018)

In this Letter we report the measurement of a pseudo-temperature 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 an effective temperature emerges (a dynamical temperature \(T_{\text{dyn}}\)) whose ratio with the equilibrium temperature \(T_{\text{eq}}\) depends on the particle density. We compare the results for the Fluctuation-Dissipation Ratio (FDR) \(T_{\text{dyn}}/T_{\text{eq}}\) at several densities with the outcomes of Edwards’ approach at the corresponding densities. It turns out that the FDR and the so-called Edwards’ ratio coincide at several densities (very different ages of the system), opening in this way the door to experimental checks as well as theoretical constructions.(PACS: 05.70.Ln, 05.20.-y, 45.70.Cc)

The study of compact granular matter through statistical physics tools is the subject of a sustained interest \([1]\). Granular media enter only partially in the framework of equilibrium statistical mechanics and their dynamics constitutes a very complex problem of non-equilibrium, which poses novel questions and challenges to theorists and experimentalists. The very possibility to construct a coherent statistical mechanics for these systems is still 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 non-thermal character of these systems: thermal energy is so negligibly small with respect to other energy contributions (e.g. potential energy) that for all the 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 it 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 non-thermal systems.

A very ambitious approach, in this direction, has been put forward by S. Edwards and co-workers \([3, 4]\), 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 \(S_{\text{edw}}\), given by the logarithm of the number of blocked configurations of given volume, energy, etc., and its corresponding density \(s_{\text{edw}} = S_{\text{edw}}/N\). Associated with this entropy are the state variables such as ‘compactivity’ \(X^{-1} = \frac{\partial}{\partial E} S_{\text{edw}}(V)\) and ‘temperature’ \(T^{-1} = \frac{\partial}{\partial S_{\text{edw}}}(E)\).

Very recently, important progresses in this direction have 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 \([3, 5]\); it was used to show that the outcome of the aging dynamics of the Kob-Andersen model (a kinetically constrained lattice gas model) was 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 \([6]\), and for sheared hard spheres \([6]\).

In this Letter we focus on the definition of a pseudo-temperature for granular media on the basis of the Fluctuation-Dissipation relations in the out-of-equilibrium, aging, dynamics of a model system \([6]\), and on its relation to Edwards’ measure. From the violation of the Fluctuation-Dissipation Theorem an effective temperature emerges (from now onward indicated as dynamical temperature \(T_{\text{dyn}}\)) whose ratio with the equilibrium temperature \(T_{\text{eq}}\) depends on the particle density. We compare the results for the Fluctuation-Dissipation Ratio (FDR) \(T_{\text{dyn}}/T_{\text{eq}}\) at several densities with the outcomes of Edwards’ approach at the corresponding densities. It turns out that the FDR and the so-called Edwards’ ratio coincide at several densities (very different ages of the system), opening in this way 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 11, 12. On the other hand, recent works on the possibility of a dynamical definition of temperature have focused on sheared, stationary systems 13, 14. 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 (non-stationary) systems.

The model we consider is a version of the “Tetris” model 15, which has been shown to reproduce several features of granular media like aging 16, 17, memory 18, self-structuring 19 etc. In the framework of this model, some of us have already provided one of the first evidences of the validity of Edwards’ measure 20.

We focus in particular on an homogeneous system with no preferential direction in order to avoid any kind of instability or large-scale structure formation 21. The case with gravity which imposes a preferential direction will be discussed elsewhere 22. In the version of the model we use, “T”-shaped particles diffuse on a square lattice, with the only constraint 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 $\frac{d}{2}$, where $d$ sets the bond size on the square lattice). The maximum density allowed is then $\rho_{max} = 2/3$. This model represents a clear example of a non-thermal 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, allowing 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 Bortz-Kalos-Lebowitz algorithm 19) where the essential ingredient is the updating of a list of mobile particles (whose number is $n_{mob}$). At each time step one selects a mobile particle and move it in the direction chosen only if no violation of the constraints occurs. The time is incremented of an amount $\Delta t = 1/n_{mob}$. We refer to 18 for the details of the fast algorithm.

We have simulated lattices of linear size $L = 50, 100, 200$, 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 $\rho(t)$, 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

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

where $N$ is the number particles present in the system at time $t_w$, $r_i$ is the coordinate $(x, y)$ of the $i$-th 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 $p = \frac{1}{2}$ to $p' = \frac{1}{2} + f^w \cdot \epsilon$, where $f^w = \pm 1$ is a random variable associated to each grain independently for each possible direction $(r = x, y)$, and $\epsilon$ represents the perturbation strength. For a constant field we obtain (see also 21, 22, 23):

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

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

If the system was in equilibrium we would expect $B$ and $\chi$ to be linearly related by

$$\chi(t + t_w, t_w) = \frac{X_{dyn}}{T_d} B(t + t_w, t_w), \quad (1)$$

where $X_{dyn}$ 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 24, then in various simulations 21, 22 how in several aging systems violations from (1) reduce to the occurrence of two regimes: a quasi-equilibrium regime with $X_{dyn} = 1$ (and time-translation invariance) for “short” time separations ($t \ll t_w$), and the aging regime with $X_{dyn} \leq 1$ for large time separations. This second slope is typically referred to as a dynamical temperature $T_{dyn} \geq T^{eq}_d$ such that $X_{dyn} = T_d^{eq}/T_{dyn}$ 23.

In our case, as the density increases, an aging behaviour is obtained: the system falls out of equilibrium and $\rho_{mob}(t)$ gets smaller than the corresponding value at equilibrium 6. Accordingly, violations of (1) 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 behaviour for $\chi$ and $B$; this is the so-called regime of interrupted aging which features an increase of $\rho_{mob}$ to its equilibrium value and a single linear relation for the $\chi$ vs. $B$ parametric plot. These measures therefore give us the value of the equilibrium fluctuation-dissipation ratio, $T_d^{eq}$, which does actually 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 behaviour and the $\chi$ vs. $B$ parametric plots, displayed in figure 1, show two different linear behaviours: after a first quasi-equilibrium regime in which the plot has slope $T_d^{eq}$, a violation of FDT is observed, with the existence of a dynamical temperature $T_d^{dyn}$ which depends on $t_w$ and therefore on the density. We obtain in particular $X_{dyn}^1 = 0.646 \pm 0.002$, $X_{dyn}^2 = 0.767 \pm 0.005$, $X_{dyn}^3 = 0.784 \pm 0.005$ at $t_w = 10^4$, $t_w = 3 \cdot 10^4$, and $t_w = 5 \cdot 10^4$.

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 procedure then yields configurations and therefore Edwards’ ratio (as in [4, 5]), we measure the ratio of the slopes (that we denote as Edwards’ ratio)

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

which is plotted in figure 2. This ratio approaches 1 as $\rho \rightarrow 2/3$, 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: $\rho_1 \approx 0.596$ for $t_w = 10^4$, $\rho_2 \approx 0.603$ for $t_w = 3.10^4$, and $\rho_3 \approx 0.605$ for $t_w = 10^5$. On the other hand, the evolution of the density of the system during the measurements is reported in figure 3.

![FIG. 1: Einstein relation in the Tetris model: plot of the mobility $\chi(t_w + t, t_w)T_d^{eq}$ vs. the mean-square displacement $B(t_w + t, t_w)$, for $t_w = 10^4$ and $t_w = 3 \cdot 10^4$. The unitary slope of the full straight line corresponds to the equilibrium case, obtained for the dynamics at constant density (interrupted aging).](image1)

![FIG. 2: Edwards’ ratio $X_{Edw}$ as a function of density. The horizontal lines correspond to the dynamical ratios $X_{dyn}$, measured (from bottom to top) at $t_w = 10^4$, $3 \cdot 10^4$, $5 \cdot 10^4$ and determine the values $\rho_1 \approx 0.596$, $\rho_2 \approx 0.603$, $\rho_3 \approx 0.605$, to be used in the comparison with the results reported in Fig. 3.](image2)

![FIG. 3: The last column reports the density intervals explored during the compaction dynamics (starting from the times where deviations from equilibrium become evident) for $t_w = 10^4$, $3 \cdot 10^4$, $5 \cdot 10^4$.](image3)

![TABLE I: Fluctuation-Dissipation Ratio ($X_{dyn}$) as obtained from numerical data fits with the corresponding densities obtained from figure 1. The last column reports the density intervals explored during the compaction dynamics (starting from the times where deviations from equilibrium become evident) for $t_w = 10^4$, $3 \cdot 10^4$, $5 \cdot 10^4$.](table1)

| $t_w$ (density) | $X_{dyn}$ | $\rho$ (density interval) |
|-----------------|-----------|---------------------------|
| $10^4$          | 0.646     | 0.596, 0.597              |
| $3 \cdot 10^4$  | 0.767     | 0.603, 0.605              |
| $5 \cdot 10^4$  | 0.784     | 0.605, 0.606              |
density increases, the measured dynamical temperature decreases, following closely the ratio between the equilibrium and the Edwards’ entropies, the latter being obtained through a flat sampling of blocked configurations. While Edwards’ proposal is supposed to be only valid asymptotically, i.e. when one-time quantities are almost stationary, our study clearly shows that it actually yields good results even in a pre-asymptotic regime, when the density is still evolving a lot.

Two remarks are in order. It is interesting to investigate the limits of validity of Edwards’ approach. Though in this letter we have shown that Edwards’ measure works nicely in the idealized case of a homogeneously compacting system, it is important to consider the case of a compacting system under gravity, i.e. with a preferential direction. We shall report about this in [18]. Another crucial point concerns the fact that the dynamically defined effective temperature could a priori depend on the observables used for the measure of Fluctuation-Dissipation relations. Its interpretation as a temperature in a thermodynamical sense would then be questioned. While the effective temperature is known to be observable independent for mean-field models, this question has been addressed only recently in realistic models: two recent studies on sheared (stationary) thermal [12] or athermal [13] systems show the consistency of various definitions [24]. Our results complement these studies by allowing to relate the value of $T_{\text{dyn}}$ to a static measure. Moreover, the observable-independence character of $T_{\text{dyn}}$ in our case will be checked in [13], by considering systems consisting of 2 types of particles. In this respect, the presence of a preferential direction could imply limitations; for sheared, stationary systems, a preferential direction exists, but only measures along orthogonal directions have been performed [8, 12, 13, 25]. Acknowledgments This work has been partially supported by the European Network-Fractals under contract No. FM-RXCT980183.

[1] Physics of Dry Granular Media (eds. Herrmann, H. J., Hovi, J.-P., and Luding, S.) 553-553 (Kluwer Academic, Dordrecht, The Netherlands, 1998).
[2] S.F. Edwards, in: Granular Matter: An Interdisciplinary Approach, A. Mehta, Ed. (Springer-Verlag, New York, 1994), and references therein.
[3] A. Mehta, R.J. Needs, S. Dattagupta, J. Stat. Phys. 68, 1131 (1992).
[4] A. Barrat, J. Kurchan, V. Loreto, Phys. Rev. Lett. 85, 5034 (2000).
[5] A. Barrat, J. Kurchan, V. Loreto, M. Sellitto, Phys. Rev. E 63, 051301 (2001).
[6] J.J. Brey, A. Prados and B. Sanchez-Rey, Phys. Rev. E 60 (1999) 5685; Physica A275 (2000) 310.
[7] D. S. Dean and A. Lefèvre, The Steady State of the Tapped Ising Model Proc. Workshop on “Challenges in granular physics”, ICTP Trieste, 7-12 August 2001, and references therein.
[8] H. Makse and J. Kurchan, 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, cond-mat/0107134.
[12] L. Berthier and J.L. Barrat, cond-mat/0110257.
[13] I.K. Ono, C.S. O’Hern, S.A. Langer, A.J. Liu and S.R. Nagel, cond-mat/0110276.
[14] M. Nicodemi and A. Coniglio, Phys. Rev. Lett. 82, 916 (1999).
[15] A. Barrat and V. Loreto, J. Phys. A: Math. Gen. 33, 4401 (2000).
[16] A. Barrat, V. Loreto, Europhys. Lett. 53, 297 (2001).
[17] 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, Phys. Rev. Lett. 84, 1039 (2000).
[18] V. Colizza, V. Loreto and A. Barrat, in preparation (2001).
[19] A. Bortz, M.H. Kalos and J.L. Lebowitz, J. Comp. Phys. 17, 10 (1975).
[20] L.F. Cugliandolo, J. Kurchan, Phys. Rev. Lett. 71, 173 (1993), J. Phys. A 27, 5749 (1994).
[21] G. Parisi, Phys. Rev. Lett. 79, 3660 (1997).
[22] W. Kob and J.L. Barrat, Europhys. Lett. 46, 637 (1999).
[23] L.F. Cugliandolo, J. Kurchan, L. Peliti, Phys. Rev. E 55, 3898 (1997).
[24] The models considered in [12, 13] are sheared, and therefore present a preferred direction. However the observables under investigation concern only the other directions.
[25] J.-L. Barrat and L. Berthier, Phys. Rev. E 63, 012503 (2001).