Emergence of macroscopic temperatures in systems that are not thermodynamical microscopically: towards a thermodynamical description of slow granular rheology

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Jorge Kurchan

PMMH Ecole Supérieure de Physique et Chimie Industrielles, 10, rue Vauquelin,
75231 Paris Cédex 05, France

Abstract.   A scenario for systems with slow dynamics is characterized by stating that there are several temperatures coexisting for the sample, with a single temperature shared by all observables at each (widely separate) timescale.

  In preparation for the study of granular rheology, we show within this framework that glassy systems with driving and friction that are generic and do not correspond to a thermal bath—and whose microscopic 'fast' motion is hence not thermal—have a well-defined macroscopic temperature associated with the slow degrees of freedom.

  This temperature is what a thermometer coupled to the system will measure if tuned to respond to low frequencies, and, since it can be related to the number of stationary configurations, it is the formalization of Edwards' 'compactivity' ideas.

1. Introduction

Granular matter set into motion by shearing, shaking, or tapping is one of the most interesting cases of macroscopic out-of-equilibrium systems. Given a granular system subjected to some form of power input that makes it perform stationary flow on average, a very natural question that arises is that of to what extent it resembles a thermodynamic system of interacting particles such as a liquid.

  More specifically, many attempts have been made to define a 'granular temperature' (see e.g. [1, 2]). In order to deserve its name, a temperature has to play the role of deciding the direction of heat flow: it must be connected to a form of the *zeroth* law. In order to pursue this line, however, one has to somehow take care of the characteristics of granular flow that distinguish it from usual kinetic theory:

 (1) Energy is not conserved, and, more generally, the motion does not have the very strong phase-space volume-conservation properties typical of Hamilton's equations. The dissipation is due to friction which is in general not linear in the velocity, and dependent upon the relative positions of the particles.
 (2) Power is supplied by tapping (which may be periodic in time) or by shearing, a mechanism very different from that of the 'collisions' of a thermal bath.

  Under these circumstances, there is no reason why the observables should be related to a Gibbs (or equivalent) ensemble, and the possibility of having thermodynamic concepts seems lost.

In this paper we shall consider situations with shear and friction, in the limit of weak shear. The effect of a coherent 'tapping' will be discussed in further work [3]. In this limit of 'slow rheology', it will turn out that even though the rapid motion cannot be associated with thermal motion, there appears for the slow flow a natural temperature playing the usual role in thermometry and thermalization [4].

The computation presented here can be done in a wide range of approximation schemes consisting in resumming a perturbative expression for the dynamics in several forms—and to higher and higher levels of approximation—in particular, the so-called mode-coupling approximation. Here, for concreteness, I will carry it through for a simple model for which the (single-mode) mode-coupling approximation is exact.

2. Multiple thermalization in aging and rheology

Granular systems have been recognized as being closely related to glassy systems [5]. Accordingly, several recent developments and models have been borrowed from the field of glasses to help in understanding their properties [12].

A picture has arisen in the last few years for aging or *gently* driven glasses involving multiple thermalizations at widely separated timescales (see [6] for a review). In the simplest scheme, the situation is as follows: given any two observables A and B belonging to the system, define the correlation function as

$$\langle A(t)B(t') \rangle = C_{AB}(t, t') \tag{1}$$

and the response of A to a field conjugate to B by

$$\frac{\delta}{\delta h_B(t')} \langle A(t) \rangle = R_{AB}(t, t'). \tag{2}$$

For a pure relaxational (undriven) glass, the correlation breaks up into two parts:

$$C_{AB}(t, t') = C_{AB}^F(t - t') + \tilde{C}_{AB}\left(\frac{h(t')}{h(t)}\right) \tag{3}$$

with h the *same* growing function for all observables A, B. The fact that $C_{AB}(t, t')$ never becomes a function of the time differences means that the system is forever out of equilibrium: it *ages*. If instead the glass is gently driven (with driving forces proportional to, say, ϵ), aging may stop, and we have

$$C_{AB}(t, t') = C_{AB}^F(t - t') + \tilde{C}_{AB}\left(\frac{t - t'}{\tau_0}\right) \tag{4}$$

where τ_0 is a timescale that diverges as ϵ goes to zero.

In the long-time limit and in the small-drive limit, the timescales become very separate. When this happens, it turns out that the responses behave as follows:

$$R_{AB}(t, t') = \beta \frac{\partial}{\partial t'} C_{AB}^F + \beta^* \frac{\partial}{\partial t'} \tilde{C}_{AB} \tag{5}$$

in the aging and the driven case.

The fast degrees of freedom behave as if thermalized at the bath temperature β. On the other hand, the effective, system-dependent temperature $T^* = 1/\beta^*$ does indeed deserve its name: it can be shown [7–9] that it is what a 'slow' thermometer measures, and it controls the heat flow and the thermalization of the slow degrees of freedom. It is *the same* for any two observables at a given timescale, whether the system is aging or gently driven. Furthermore, it is *macroscopic*: it remains non-zero in the limit in which the bath temperature is zero.

If the system is not coupled to a true thermal bath, but energy is supplied by shaking and shearing, while it is dissipated by a non-linear complicated friction, there is no bath temperature β. What will be argued in what follows is that even so, the 'slow' temperature β^* survives despite the fact that the fast motion is not thermal in that case. Indeed, if we have correlation having fast and slow components:

$$C_{AB}(t, t') = C_{AB}^F(t, t') + \hat{C}_{AB}^S(t, t') \tag{6}$$

then the response is of the form

$$R_{AB}(t, t') = R_{AB}^F(t, t') + \beta^* \frac{\partial}{\partial t'} \hat{C}_{AB}^S(t, t') \tag{7}$$

with the fast response $R_{AB}^F(t, t')$ bearing no general relation to the fast correlation $C_{AB}^F(t, t')$.

The effective 'slow' temperature so defined is then found to be directly related to Edwards' compactivity [2], but, in the spirit of reference [10], in the context of slowly moving rather than stationary systems [11]. It seems also closely related to the macroscopic temperature that drives activated processes in the SGR model [12].

3. A simple example

For concreteness, let us consider a variation of the standard mean-field glass model [6, 13]. The variables are x_i, $i = 1, \ldots, N$, and are subject to an equation of motion:

$$m\ddot{x}_i + \frac{\delta E(\boldsymbol{x})}{\delta x_i} + \Omega x_i = -\epsilon f_i^{\text{'shear'}}(\boldsymbol{x}) - f_i^{\text{'friction'}}(\dot{\boldsymbol{x}}). \tag{8}$$

The left-hand side is just Newtonian dynamics (with Ω possibly time dependent), with a 'glassy' potential which we can take, for example, as

$$E(\boldsymbol{x}) = \sum J_{ijk} x_i x_j x_k \tag{9}$$

where the J_{ijk} is a symmetric tensor of random quenched variables of variance $1/N^2$. These terms correspond to the p-spin glass [13]. It was realized some ten years ago that this kind of model constitutes a mean-field 'caricature' of fragile glass [14], and in particular its dynamics yields above the glass transition the simplified mode-coupling equations [15].

On the right-hand side of equation (8) we have added two terms that mimic granular experiments. The forces f_i do not derive from a potential; for example [3, 16],

$$f_i^{\text{'shear'}}(\boldsymbol{x}) = K_{jk}^i x_j x_k \tag{10}$$

with K_{jk}^i a *non-symmetric* tensor with random elements with variance $1/N$. They pump energy into the system, and hence play a role similar to shearing. *All of our discussion will be restricted to weak driving, i.e. ϵ small.* For the friction terms we can take, instead of a linear term $\propto \dot{x}_i$, a more complicated *odd* function $f_i^{\text{'friction'}} = f^{\text{'friction'}}(\dot{x}_i)$.

The equations for the correlation

$$C(t, t') = \frac{1}{N} \sum \langle x_i(t) x_i(t') \rangle$$

and response

$$R(t, t') = \frac{1}{N} \sum \delta \langle x_i(t) \rangle / \delta h_i(t')$$

can be exactly solved in the large-N limit. One may do this by reducing the system to a self-consistent single-site equation [17]:

$$m\ddot{x} + \Omega x = -\epsilon f^{\text{'shear'}}(t) - f^{\text{'friction'}}(\dot{x}) + 6 \int^t dt'\, C(t, t') R(t, t') x(t') + \rho(t). \tag{11}$$

$f^{\text{`shear'}}(t)$ and $\rho(t)$ are independent coloured Gaussian noises that satisfy

$$\langle f^{\text{`shear'}}(t) f^{\text{`shear'}}(t')\rangle = \langle \rho(t)\rho(t')\rangle = 3C^2(t,t'). \tag{12}$$

Equation (11) is supplemented by the self-consistency conditions

$$\langle x(t)x(t')\rangle = C(t,t') \qquad R(t,t') = \frac{\delta\langle x(t)\rangle}{\delta h(t')} \tag{13}$$

where $h(t)$ is a field that acts additively in (11).

We now perform the usual step of separating 'fast' and 'slow' functions. Accordingly, we put

$$\begin{aligned} C(t,t') &= C_F(t,t') + C_S(t,t') & R(t,t') &= R_F(t,t') + R_S(t,t') \\ f^{\text{`shear'}} &= f_F^{\text{`shear'}} + f_S^{\text{`shear'}} & \rho &= \rho_F + \rho_S. \end{aligned} \tag{14}$$

The additive separation is such that in the region of large time differences, $C_F(t,t')$ and the integral of $R_F(t,t')$ tend to zero, and the induced noises are now divided into fast and slow:

$$\begin{aligned} \langle f_F^{\text{`shear'}}(t) f_F^{\text{`shear'}}(t')\rangle &= \langle \rho_F(t)\rho_F(t')\rangle = 3C_F^2(t,t') \\ \langle f_S^{\text{`shear'}}(t) f_S^{\text{`shear'}}(t')\rangle &= \langle \rho_S(t)\rho_S(t')\rangle = 3C_S^2(t,t'). \end{aligned} \tag{15}$$

We can now rewrite the single-site equation (11) in the following way:

$$m\ddot{x} + \Omega x = -\epsilon f_F^{\text{`shear'}}(t) - f^{\text{`friction'}}(\dot{x}) + 6\int^t dt'\, C_F(t,t') R_F(t,t') x(t') + \rho_F(t) + Z(t) \tag{16}$$

where

$$Z(t) = -\epsilon f_S^{\text{`shear'}}(t) + 6\int^t dt'\, C_S(t,t') R_S(t,t') x(t') + \rho_S(t). \tag{17}$$

Consider equation (16): it describes a single degree of freedom which has non-linear friction and a (short) memory kernel, plus a *slowly varying* field $Z(t)$. Upon the assumption of large separation of timescales (which will be valid if the system is weakly sheared and 'old'), we can treat $Z(t)$ as adiabatic. However, because of the absence of detailed balance, we know that the distribution for fixed Z is *non-Gibbsean*. The fast correlation and response functions will be of the forms $C_F(t,t') = C_F(t-t')$ and $R_F(t,t') = R_F(t-t')$, but we cannot say anything in general about their relation. The average of $\langle\langle x\rangle\rangle_Z$ over an interval of time large compared to the fast relaxation (the range of C_F and R_F) is a certain function of Z:

$$\langle\langle x\rangle\rangle_Z = \frac{\partial F(Z)}{\partial Z} \tag{18}$$

which defines the single-variable function $F(Z)$.

We now turn to the slow evolution. Because the memory kernels in equation (17) are slowly varying and smooth, we can substitute for x its average $\langle\langle x\rangle\rangle_Z$. We hence have

$$Z(t) = -\epsilon f_S^{\text{`shear'}}(t) + 6\int^t dt'\, C_S(t,t') R_S(t,t') \frac{\partial F(Z)}{\partial Z}(t') + \rho_S(t) + h^{\text{adiab}}(t) \tag{19}$$

where we have explicitly made the slow component a field acting additively in (11). The self-consistency equations now read

$$C_S(t,t') = \left\langle \frac{\partial F(Z)}{\partial Z}(t) \frac{\partial F(Z)}{\partial Z}(t') \right\rangle \qquad R_S(t,t') = \frac{\delta}{\delta h^{\text{adiab}}(t')} \left\langle \frac{\partial F(Z)}{\partial Z}(t) \right\rangle. \tag{20}$$

Equations (19) and (20) describe the slow part of the evolution. The only input of the fast equations is through the function $F(Z)$. The manner of solution depends little on the fact that

the 'fast' evolution is not thermal, and is by now standard. Here I sketch the steps [18] for completeness. Our aim is to show that they admit in the small-ϵ limit a solution of the form

$$C_S(t, t') = \tilde{C}\left(\frac{h(t')}{h(t)}\right) \qquad R_S(t, t') = \beta^* \frac{\partial}{\partial t'} \tilde{C}\left(\frac{h(t')}{h(t)}\right) \qquad (21)$$

where β^* is the effective temperature that emerges for the slow dynamics, to be determined by the matching with the 'fast' time sector. To show this, we first write $\tau = \ln(h(t))$, $\tau' = \ln(h(t'))$, etc, and put

$$
\begin{aligned}
C_S(t, t') &= \hat{C}(\tau - \tau') \\
R_S(t, t') &= \beta^* \frac{\partial}{\partial \tau'} \hat{C}(\tau - \tau') \\
Z(t) &= \hat{Z}(\tau).
\end{aligned}
\qquad (22)
$$

Equations (19) and (20) now take the form, in the $\epsilon \to 0$ limit,

$$\hat{Z}(\tau) = -\epsilon f_S^{\text{'shear'}}(\tau) + 6\beta^* \int^\tau d\tau' \, \hat{C}(\tau - \tau') \hat{C}'(\tau - \tau') \frac{\partial F(\hat{Z})}{\partial \hat{Z}}(\tau') + \rho_S(\tau) + h^{\text{adiab}} \qquad (23)$$

where we have explicitly made the slow component a field acting additively in (11). The self-consistency equations read

$$\hat{C}(\tau - \tau') = \left\langle \frac{\partial F(\hat{Z})}{\partial \hat{Z}}(\tau) \frac{\partial F(\hat{Z})}{\partial \hat{Z}}(\tau') \right\rangle \qquad (24)$$

and

$$\beta^* \frac{\partial}{\partial \tau'} \hat{C}(\tau - \tau') = \frac{\delta}{\delta h^{\text{adiab}}(\tau')} \left\langle \frac{\partial F(\hat{Z})}{\partial \hat{Z}}(\tau) \right\rangle. \qquad (25)$$

To prove that (22) is a solution of the system (23)–(25), and hence that (21) is a solution of (19) and (20), we can proceed as follows: we introduce an infinite set of auxiliary variables $l_i(\tau)$ and a set of dynamical variables y_i satisfying an ordinary Langevin equation with inverse temperature β^*:

$$\left[m_j \frac{d^2}{d\tau^2} + \Gamma_j \frac{d}{d\tau} + \Omega_j \right] y_j + l_j(\tau) = \Delta_j y_j + l_j(\tau) = \xi_j(\tau) - \partial F\left(\sum_j A_j y_j\right) \Big/ \partial y_j \qquad (26)$$

with

$$\langle \xi_i(\tau) \xi_j(\tau_w) \rangle = 2T^* \Gamma_j \delta_{ij} \delta(\tau - \tau_w). \qquad (27)$$

We can now choose the A_j and the l_j such that

$$
\begin{aligned}
\Delta_j^{-1} \sum_j A_j \xi_j(t) &= \rho(t) \\
\sum_j A_j^2 \Delta_j^{-1} &= \hat{C}'(\tau) \Theta(\tau) \\
\sum_j A_j \Delta_j^{-1} l_j(\tau) &= h^{\text{adiab}}(\tau)
\end{aligned}
\qquad (28)
$$

and check that the quantity $\sum_j A_j y_j$ obeys the same equation of motion as $Z(\tau)$.

Because the problem reduced to an ordinary (not glassy!) Langevin equation, we can be confident that the system thermalizes at temperature $T^* = 1/\beta^*$, and hence guarantee that the *ansatz* closes.

We have followed essentially the same steps as in the treatment of a glassy model coupled to a 'good' heat bath. Here, instead of having two timescales each with its own temperature, we have a temperature associated only with the low-frequency motion.

4. Conclusions

It has been recognized for some time that granular systems bear a strong resemblance to glassy systems at essentially zero temperature. In order to introduce some agitation, both tapping and shearing have often been introduced. This certainly makes sand look more like a fluid, but at the same time poses the problem of introducing (and dissipating) energy in a manner that is quite different from that which is operative in a thermal bath.

We have shown in this paper that, at least within an approximation scheme and for *slowly flowing systems*, one can still introduce thermodynamic concepts—provided that one attempts to apply them only to the low-frequency motion.

For very small power input, it turns out that the fluctuation-dissipation temperature of the slow degrees of freedom coincides in these models with Edwards', defined on the basis of the logarithm of the number of stable configurations [9]. For stronger driving power, an analogous definition needs the counting of stable states, each composed of many configurations.

Acknowledgment

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