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

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(March 24, 2022)

Abstract

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

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 to 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 formalisation of Edwards’ ‘compactivity’ ideas.

I.

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 to what extent it resembles a thermodynamic system of interacting particles such as, for example, a liquid.

More specifically, many attempts have been made to define a ‘granular temperature’ (see e.g. [1]). 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 zero-th 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 manner 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. 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 thermalisation.

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.

**Multiple Thermalisation in Aging and Rheology**

Granular systems have been recognised as being closely related to glassy systems. Accordingly, several recent developments and models have been borrowed from the field of glasses to understand their properties.

A picture has arisen in the last few years for aging or gently driven glasses involving multiple thermalisations at widely separated timescales (see 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:

\[
\langle A(t)B(t') \rangle = C_{AB}(t, t')
\]

and the response of \( A \) to a field conjugate to \( B \):

\[
\frac{\delta}{\delta h_B(t')} \langle A(t) \rangle = R_{AB}(t, t')
\]

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

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

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, \( \epsilon \)), aging may stop, and we have:

\[
C_{AB}(t, t') = C_{AB}^F(t - t') + \tilde{C}_{AB} \left( \frac{t - t'}{\tau_o} \right)
\]
where \( \tau_o \) is a time scale that diverges as \( \epsilon \) goes to zero.

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

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

in the aging and the driven case.

The fast degrees of freedom behave as if thermalised at the bath temperature \( \beta \). On the other hand, the effective, system-dependent temperature \( T^* = 1/\beta^* \) indeed deserves its name: it can be shown that it is what a ‘slow’ thermometer measures, and it controls the heat flow and the thermalisation 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 nonlinear complicated friction, there is no bath temperature \( \beta \). What will be argued in what follows is that even so, the ‘slow’ temperature \( \beta^* \) survives despite the fact that the fast motion is not thermal in that case. Indeed, if we have correlation having fast and slow components:

\[
C_{AB}(t, t') = C_{AB}^F(t, t') + \hat{C}_{AB}^S(t, t')
\]

the response is of the form:

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

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

The effective ‘slow’ temperature so defined is then found to be directly related to Edwards’ compactivity, but, in the spirit of Ref., in the context of slowly moving rather than stationary systems. It seems also closely related to the macroscopic temperature driving activated proceses in the SGR model.

A Simple Example

For concreteness, let us consider a variation of the standard mean-field glass mode. The variables are \( x_i, i = 1, ..., N \), and are subject to an equation of motion:

\[
m \ddot{x}_i + \frac{\delta E(x)}{\delta x_i} + \Omega x_i = -\epsilon f_i \text{‘shear’}(x) - f_i \text{‘friction’}(\dot{x})
\]

The left hand side is just Newtonian dynamics (with \( \Omega \) possibly time-dependent), with a ‘glassy’ potential which we can take, for example, as:

\[
E(x) = \sum J_{ijk} x_i x_j x_k
\]

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. It was realised some ten years ago that this kind of
model constitutes a mean-field caricature of fragile glasses, and in particular its dynamics yields above the glass transition the simplified mode-coupling equations.

On the right hand-side of Eqn. (1.10) we have added two terms that mimic granular experiments. The forces \( f_i \) do not derive from a potential, for example:

\[
f'_i(x) = K_{jk} x_j x_k
\]

with \( K_{jk} \) 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 our discussion will be restricted to weak driving, i.e. \( \epsilon \) small. For the friction terms we can take, instead of a linear term \( \alpha \dot{x}_i \), a more complicated odd function \( f'_i = f^{\text{friction}}(\dot{x}_i) \).

These equations for the correlation \( C(t,t') = \frac{1}{N} \sum \langle x_i(t)x_i(t') \rangle \) and response \( R(t,t') = \frac{1}{N} \sum \delta(x_i(t))/\delta h_i(t') \) can be exactly solved in the large \( N \) limit. One may do so by reducing the system to a self-consistent single-site equation:

\[
m\ddot{x} + \Omega x = -\epsilon f'_i(x) + f^{\text{friction}}(\dot{x}) + 6\int dt' C(t,t') R(t,t') x(t') + \rho(t)
\]

Equation (1.11) is supplemented by the self-consistency conditions

\[
\langle x(t)x(t') \rangle = C(t,t') \quad R(t,t') = \frac{\delta(x(t))}{\delta h(t')}
\]

where \( h(t) \) is a field that acts additively in (1.11).

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

\[
C(t,t') = C_F(t,t') + C_S(t,t') \quad R(t,t') = R_F(t,t') + R_S(t,t')
\]

\[
f'_i = f'_i + f'_i \quad \rho = \rho_F + \rho_S
\]

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:

\[
\langle f'_F(x) f'_F(x) \rangle = \langle \rho_F(t) \rho_F(t) \rangle = 3C_F^2(t,t')
\]

\[
\langle f'_S(x) f'_S(x) \rangle = \langle \rho_S(t) \rho_S(t) \rangle = 3C_S^2(t,t')
\]

We can now rewrite the single-site equation (1.11) in the following way:

\[
m\ddot{x} + \Omega x = -\epsilon f'_F(x) - f^{\text{friction}}(\dot{x}) + 6\int dt' C_F(t,t') R_F(t,t') x(t') + \rho_F(t) + Z(t)
\]
where:

$$Z(t) = -\epsilon f_s^{\text{\textquoteleft shear\textquoteright}}(t) + 6 \int^t dt' C_s(t, t') R_s(t, t') x(t') + \rho_s(t)$$  \hfill (1.17)$$

Consider equation (1.16): it describes a single degree of freedom which has nonlinear friction and a (short) memory kernel, plus a \textit{slowly varying} field \(Z(t)\). Upon the assumption of large separation of timescales (which will be valid if the system is weakly sheared and \textquoteleft old\textquoteright{}), we can treat \(Z(t)\) as adiabatic. However, because of the absence of detailed balance, we know that the distribution for fixed \(Z\) is \textit{non-Gibbsean}. The fast correlation and response functions will be of the form \(C_F(t, t') = C_F(t - t')\) 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 \(Z\):

$$\langle\langle x \rangle\rangle_{Z} = \frac{\partial F(Z)}{\partial Z}$$  \hfill (1.18)$$

which defines the single variable function \(F(Z)\).

We now turn to the slow evolution. Because the memory kernels in equation (1.17) are slowly varying and smooth, we can substitute \(x\) by its average \(\langle\langle x \rangle\rangle_{Z}\). We hence have:

$$Z(t) = -\epsilon f_s^{\text{\textquoteleft shear\textquoteright}}(t) + 6 \int^t dt' C_s(t, t') R_s(t, t') \frac{\partial F(Z)}{\partial Z}(t') + \rho_s(t) + h_{\text{adiab}}(t)$$  \hfill (1.19)$$

where we have explicitated the slow component a field acting additively in (1.11). The self-consistency equations now read:

$$C_s(t, t') = \langle \frac{\partial F(Z)}{\partial Z}(t) \frac{\partial F(Z)}{\partial Z}(t') \rangle; \quad R_s(t, t') = \frac{\delta}{\delta h_{\text{adiab}}(t')} \langle \frac{\partial F(Z)}{\partial Z}(t) \rangle$$  \hfill (1.20)$$

Equations (1.19) and (1.20) 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 \textquoteleft fast\textquoteright{} evolution is not thermal, and is by now standard. Here I sketch the steps \[\text{for completeness. Our aim is to show that they admit in the small } \epsilon \text{ limit a solution of the form:}\]

$$C_s(t, t') = \tilde{C} \left( \frac{h(t')}{h(t)} \right) \quad ; \quad R_s(t, t') = \beta^* \frac{\partial}{\partial t'} \tilde{C} \left( \frac{h(t')}{h(t)} \right)$$  \hfill (1.21)$$

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

$$C_s(t, t') = \tilde{C}(\tau - \tau') \quad \quad ; \quad \quad R_s(t, t') = \beta^* \frac{\partial}{\partial t'} \tilde{C}(\tau - \tau')$$

$$Z(t) = \tilde{Z}(\tau)$$  \hfill (1.22)$$

Equations (1.19) and (1.20) now take the form, in the \(\epsilon \to 0\) limit:
\[
\dot{Z}(\tau) = -\epsilon f_s^{\text{shear}}(\tau) + 6\beta^* \int_{\tau}^{\tau'} d\tau' \dot{C}(\tau - \tau')\dot{C}'(\tau - \tau') \frac{\partial F(\dot{Z})}{\partial \dot{Z}(\tau')} + \rho_s(\tau) + h^{\text{adiab}}
\]

where we have explicitated the slow component a field acting additively in (1.11). The self-consistency equations read:

\[
\dot{C}(\tau - \tau') = \langle \frac{\partial F(\dot{Z})}{\partial \dot{Z}(\tau)} \frac{\partial F(\dot{Z})}{\partial \dot{Z}(\tau')} \rangle
\]

and

\[
\beta^* \frac{\partial}{\partial \tau'} \dot{C}(\tau - \tau') = \frac{\delta}{\delta h^{\text{adiab}}(\tau')} \langle \frac{\partial F(\dot{Z})}{\partial \dot{Z}(\tau)} \rangle
\]

To prove that (1.22) is a solution of the system (1.23) - (1.25), and hence that (1.21) is a solution of (1.19) and (1.20) 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 \(\beta^*\):

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

with

\[
\langle \xi_i(\tau)\xi_j(\tau_w) \rangle = 2T^* \Gamma_j \delta_{ij} \delta(\tau - \tau_w)
\]

We can now choose the \(A_j\) and the \(l_j\) such that:

\[
\Delta_j^{-1} \sum_j A_j \xi_j(t) = \rho(t)
\]

\[
\sum_j A_j^2 \Delta_j^{-1} = \dot{\dot{C}}'(\tau) \Theta(\tau)
\]

\[
\sum_j A_j \Delta_j^{-1} l_j(\tau) = h^{\text{adiab}}(\tau)
\]

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 assure that the system thermalises at temperature \(T^* = 1/\beta^*\), and hence verify that the ansatz closes.

We have followed essentially the same steps as in the treatment of a glassy models coupled to a ‘good’ heat bath. Here instead of having two time scales each with its own temperature we have a temperature associated only with the low frequency motion.
Conclusions

It has been recognised for some time that granular systems bear a deep similarity with glassy systems at essentially zero temperature. In order to introduce some agitation, both tapping and shearing have been often 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 of 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 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.

Acknowledgements

I wish to thank Anita Mehta for useful comments.
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