Why Granular Media Are, After All, Thermal

Yimin Jiang\textsuperscript{1} and Mario Liu\textsuperscript{2}

\textsuperscript{1}Central South University, Changsha 410083, China
\textsuperscript{2}Theoretische Physik, Universität Tübingen, 72076 Tübingen, Germany

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Granular media are considered \textit{athermal}, because the grains are too large to display Brownian type thermal fluctuations. On the other hand, being macroscopic, every grain undergoes thermal expansion, possesses a temperature that may be measured with a thermometer, and consists of many, many internal degrees of freedom that in their sum do affect granular dynamics. Therefore, including them in a comprehensive approach to account for granular behavior entails crucial advantages. The pros and cons of thermal versus athermal descriptions are considered.

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Taking grains as athermal particles interacting via the Newtonian law with an elasto-frictional force, discrete element method (DEM) has been a success story\textsuperscript{3}.\textsuperscript{4}, to the extent that it is today the tool of choice for coming to terms with granular behavior\textsuperscript{5}.\textsuperscript{6},\textsuperscript{7}. A second success story is the granular kinetic theory\textsuperscript{8}.\textsuperscript{9},\textsuperscript{10} that also takes grains as athermal particles colliding with a restitution coefficient smaller than one. As a result – and because granular Brownian motion is imperceptibly small – it is a common place of the granular community that grains may generally be approximated as athermal particles. This believe is best reflected in athermal statistical mechanics (ASM) that defines, in addition, an entropy $S$ (as the logarithm of the number grains may be stably packed), assuming it is maximal in equilibrium, if the numbers are appropriately weighted\textsuperscript{10}–\textsuperscript{14}. (In contrast, DEM neither needs an entropy to guide the system towards the rest state, nor ever introduces it.) Being non-conserved, energy is typically discarded as a state variable. Instead, $S$ is taken to depend on the volume and force moment tensor. Force equilibrium is often assumed.

This is a leap of faith: Granular Brownian motion is small because grains are macroscopic. But there are then many, many internal microscopic degrees of freedom that one needs to make sure are irrelevant. To see whether they are, consider the textbook example of a pendulum. Its motion is given by the Newtonian force law of a mass point, including a friction term – no need to consider any microscopic degrees here. But to determine the sign of the friction, to make sure that the amplitude diminishes, one needs to consider how the total entropy, consisting mainly of microscopic degrees of freedom, increases. These are the air molecules surrounding the pendulum and the phonons in the string – also the phonons and electrons in the pendular weights, if there are two steel pendula colliding periodically. When the pendula come to a standstill hanging down, their macroscopic energy is zero, and the total entropy maximal.

If this is an apt analogy for the relation between DEM and granular statistical mechanics, if the microscopic degrees of freedom do influence the macroscopic dynamics, they must be included when calculating the entropy.

At any rate, if we consider the air or water surrounding the grains, we need to include their molecular degrees of freedom in an entropic considerations: Is it not consistent to include the inner-granular ones as well?

Doing so, helpfully, the total energy is conserved, and the thermal statistical mechanics valid – as is thermodynamics. Employing them, one finds that the grain-level energy dissipates because it is being redistributed to the microscopic degrees of freedom, and that force equilibrium holds as a result of $S$ being maximal.

We therefore submit: Granular media are not generally athermal. More specifically, taking a reduced entropy that excludes internal degrees of freedom as maximal in equilibrium, one bears a heavy burden of proof.

Two-stage irreversibility, a useful notion for coming to terms with granular thermodynamics is related to the three spatial scales of any granular media: (a) the macroscopic, (b) the mesoscopic or inter-granular, and (c) the microscopic or inner granular. Dividing all degrees of freedom into these three categories, one treats those of (a) differently from (b,c). Macroscopic degrees of freedom (the slowly varying stress, flow and density fields) are employed as state variables, but inter- and inner granular degrees of freedom are treated summarily: Only their contributions to the energy is considered and taken, respectively, as granular and true heat. One does not account for the microscopic dynamics of phonons and electrons, but takes the sum of their energy as $\int T dS$. Similarly, one does not account for the motion and deformation of every grain, only includes their fluctuating kinetic and elastic energy as granular heat $W_T$. Defining $S_g$ as the logarithms of the number of states the inter-granular degrees may be in, and $T_g \equiv \partial W_T/\partial S_g$, we again have $W_T = \int T_g dS_g$. There are a handful of macroscopic degrees of freedom (a), a large number of inter-granular ones (b), and yet many orders of magnitude more inner granular ones (c). So the statistical tendency to equally distribute the energy among all degrees of freedom implies an energy decay: $(a \to c)$ and $(a \to b \to c)$, or what
Irreversibility is implied by the three energy-decay terms \( R_g, R_s, I \) and moving grains, versions of the reduced entropy in ASM, though FDT holds in a block of copper, although it is much larger. A general principle, should not be valid in granular media: electrons in solid. So there is no reason why FDT, a general principle, should not be valid in granular media. The microscopic degrees of freedom are always to grain-level fluctuations: Thermal fluctuations are universally set to zero in DEM, and it is difficult, if at all possible, to separate both in experiments.

The fluctuation-dissipation theorem (FDT) correlates the thermal fluctuations of the microscopic degrees of freedom in equilibrium to how they return to equilibrium after having been exposed to a small applied perturbation, i.e., to the friction and dissipation that they experience. The microscopic degrees of freedom are atoms or molecules in gas and liquid, and phonons, free electrons in solid. So there is no reason why FDT, a general principle, should not be valid in granular media: FDT holds in a block of copper, although it is much larger than a grain and has even smaller Brownian motion. This remains so when one cuts the block in half, because a cut is too small and macroscopic a perturbation to appreciably affect FDT, or the linear response theory employed to deduce it. Further cuts are also allowed, as long as the pieces remain macroscopic. The link between thermal fluctuations and the return to equilibrium will not be severed — although the link may change, because the system’s hydrodynamics (such as given by GSH) does. This conclusion clearly holds for all granular media.

The Onsager relation (OR) is a direct consequence of FDT. If the latter holds, so does the former. But there is also an independent counter-argument that we need to deal with: The validity of the OR depends on the time reversal invariance of the underlying microscopic dynamics, yet grains collide inelastically and execute irreversible motion. This is why many believe OR need not hold in granular media, see [22]. This point of view again ignores the fact that grains are not elementary. The granular kinetic theory is a truncated one, and the apparent lack of time reversal symmetry is a result of this truncation. The microscopic degrees of freedom in sand obey, as everywhere else, the reversible Schrödinger equation.

OR concerns the pairwise equality (with same or opposite signs) of transport coefficients, a fact that may be verified experimentally. Although no one is capable of employing the Schrödinger equation to calculate the coefficients directly, there should be little doubt that the result will comply with the OR. Therefore, a proper calculation employing the dissipative kinetic theory must arrive at the same result. (This may not be easy, as the kinetic theory at present only considers \( R_g \), not \( R \), see Fig 1.)

More generally, OR is valid in all condensed systems: solids, superfluids, liquid crystals, because all share the same microscopic dynamics. Breaking a solid block into (macroscopic) pieces does not change this fact.

Is \( T_g \) a true temperature? Yes, \( T_g \) and \( T \) each characterizes the energy of a group of degrees of freedom, with a given rate of energy transfer between them. Usually, the degrees of freedom of two systems in thermal contact are spatially separated. In this case, they are not, which

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**Figure 1.** Dissipative processes produce either granular entropy \( S_g \), or thermal entropy \( S \). Eventually, \( S_g \) also decays to \( S \). Irreversibility is implied by the three energy-decay terms \( R, R_g, I \), being always positive. Containing all states of deformed and moving grains, \( S_g \) is a much larger quantity than various versions of the reduced entropy in ASM, though \( S_g \ll S \) still holds. The system is in equilibrium if \( S_{tot} = S + S_g \approx S \) is maximal. Maximal \( S_g \) characterizes (quasi-)equilibrium for times \( t \ll \tau \) (with \( \tau \) the time scale of \( I \)). Then conventional statistical mechanics and thermodynamics hold. Maximal \( S_g \) for \( t \to \infty \) is a novel proposition.
is the main difference. Any difficulties treating \( T_g \) as a temperature arise because one ignores \( T - 1 \) as in the cases discussed above, and it is also the reason for the failure of granular media to equilibrate, that granular temperatures of two systems in contact are different.

Given two granular systems, 1 and 2, with only 1 being excited, there are, in the steady state, four generally unequal temperatures: \( T_1^1, T_2^1, T_2^2, T_2^2 \), and an ongoing energy transfer (\( T_1^1 \rightarrow T_1^1 \), \( T_1^1 \rightarrow T_2^2 \)) and (\( T_2^2 \rightarrow T_2^2 \)). Their differences depend on details such as the restitution coefficients and the contact area. This is quite similar to four thermal systems, two large (1, 2), two small (1a, 2a), with (1a) being heated, and (1a, 1), (1a, 2a), (2a, 2) in pairwise thermal contact. All four temperatures will usually be different, and there is an ongoing energy flux.

The passive granular system 2 may serve as a thermometer if it consisted of completely elastic beads, and usually be different, and there is an ongoing energy flux.

As this expression assumes only analyticity of \( \partial w/\partial \rho \), the non-optimal energy distribution between the inter- and inner granular degrees of freedom, \( T_g - T \) relaxes until it vanishes. Now, since \( s \gg s_g \), and since any granular motion at all already implies \( T_g \neq T \), we have \( T_g - T \approx T_g \), \( s + s_g \approx s \), and this rewriting does not change anything. So we may take \( T_g \) as the relaxing quantity, with \( T_g = 0 \) replacing \( T_g = T \) at equilibrium. [This result is essential for obtaining Eq. (1).]

Formal equilibrium conditions, given in terms of the conjugate variables and valid irrespective what the actual expression for \( w = w(s, s_g, \rho, u_{ij}) \) is, are obtained by requiring \( \int s \, d^3r \) to be maximal, under the constraints of constant energy \( \int w \, d^3r \) and mass \( \int \rho \, d^3r \). In granular media, remarkably, this universally valid procedure leads to two sets of equilibrium conditions, solid- and fluid-like.

Maximizing the entropy (see [13–17] for details), we always obtain \( \nabla_i T = 0 \), and \( T_g = 0 \). Usually, \( T_g \) vanishes quickly, and if it does, the density no longer varies independently from the elastic strain, \( \delta P/\rho = -dw_{ij} \). They then share a common, solid-like equilibrium condition,

\[
\nabla_i (\pi_{ij} + P_T \delta_{ij}) = \rho \, g_i, \tag{2}
\]

where \( g_i \) is the gravitational constant, \( \pi_{ij} \) the elastic stress, \( P_T \equiv -\partial (wV)/\partial V \) the usual fluid pressure (\( V \) is the volume, and the derivative is taken at constant \( \rho V, s_{tot} V \) and \( s_g V \)). With Eq. (1) below, \( P_T \sim T_g^2 \rightarrow 0 \) is the pressure exerted by jiggling grains. Clearly, Eq. (2) expresses force balance in the jammed state.

If \( T_g \) is kept finite by continual external perturbations, the system further increases its entropy by independently varying \( \rho \) and \( u_{ij} \), to arrive at the fluid equilibrium, characterized by two conditions. The first, with respect to \( u_{ij} \), requires any shear stress to vanish and any free surface to be horizontal in equilibrium; the second is related to reversible compaction, see [19] for more details:

\[
\pi_{ij} = 0, \quad \nabla_i P_T = \rho \, g_i. \tag{3}
\]

The relation between \( T_g \) and \( s_g \): In the gaseous phase, grains have only kinetic energy, \( \frac{1}{2} T_g \) per degree of freedom. With \( N \) the number of grains, the total energy is \( W_T = \frac{3}{2} T_g N \). If the inner granular degrees of freedom may be modeled as a phonon gas, the inner energy is \( 3T N_a \) (for \( T \gg T_D \), the Debye temperature, and with \( N_a \) the number of atoms in all the grains). Assuming unrealistically that the grains maintained their integrity at arbitrarily high \( T \), they will heat up during a collision for \( T_g > T \), but cool down for \( T_g < T \), until \( T_g = T \), a result associated with the total energy being conserved.

Usually, of course, because \( T_g \gg T \), the heat transfer is accounted for by a constant restitution coefficient.

This picture becomes blurred at higher densities, breaking down completely when the contacts are enduring. Given the friction between grains, a suitable \( w(s_g) \) is difficult to obtain microscopically. Therefore, we pragmatically expand \( w \) in \( s_g \), requiring \( T_g = 0 \) to be minimal. Denoting \( w_T = w - w(T_g = 0) \), we have

\[
w_T = s_g^2/2\rho b - \rho b T_g^2/2, \quad \partial w/\partial s_g|_s = s_g/\rho b. \tag{4}
\]

As this expression assumes only analyticity of \( w \) and does not depend on interactions, it is quite general – as long as \( T_g \) is sufficiently small.

One could now find an appropriate formula interpolating between this limit and the gaseous one. But we,

Granular Thermodynamics has, as its set of state variables, first the usual ones: the density \( \rho \), the momentum density \( \rho v_i \), the total entropy \( s_{tot} \); then in addition: the granular entropy \( s_g \), the elastic strain \( u_{ij} \). (The elastic strain \( u_{ij} \) is a coarse-grained measure of the grains’ elastic deformation, and not the total strain, see [13–17].) Denoting the conserved energy density (in the rest frame, \( v_i = 0 \)) as \( w = w(s, s_g, \rho, u_{ij}) \), the conjugate variables are: \( T \equiv \partial w/\partial s_g, T_g \equiv \partial w/\partial s_g, \mu \equiv \partial w/\partial \rho, \pi_{ij} \equiv -\partial w/\partial u_{ij} \), where \( \mu \) is the chemical potential and \( \pi_{ij} \) the elastic stress. This is conveniently written as

\[
dw = Tds + T_g ds_g + \mu d\rho - \pi_{ij} du_{ij}, \tag{1}
\]

a formula valid as long as the variables are as given. Writing \( Tds + T_g ds_g = T d(s + s_g) + (T_g - T) ds_g \), we identify the first term as the equilibrium energy for \( T_g = T \), and the second as the additional contribution if \( T_g \neq T \). Characterizing the non-optimal energy distribution between the inter- and inner granular degrees of freedom, \( T_g - T \) relaxes until it vanishes. Now, since \( s \gg s_g \), and since any granular motion at all already implies \( T_g \gg T \), we have \( T_g - T \approx T_g \), \( s + s_g \approx s \), and this rewriting does not change anything. So we may take \( T_g \) as the relaxing quantity, with \( T_g = 0 \) replacing \( T_g = T \) at equilibrium.
rather more simply, employ Eq. [4] for all values of $T_g$. This works because of $T_g$’s two functions, as a measure for equilibration and as a state variable, only the second is relevant in practice: Substituting $w_T = \rho b T_g^2/2$ for $w_T = \frac{3}{2} T_k \rho / m$ implies $T_k = \frac{1}{3} m b T_g^2$ in the gaseous limit ($m$ is the average mass of a grain, $T_k$ is introduced to distinguish both). This is impermissible when one considers equilibration, as done above, because it is $T_k$ that becomes equal to $T$, not $T_g$. On the other hand, such super hot grains do not exist, and equilibration considers equilibration, as done above, because it is to distinguish both). This is impermissible when one.

Conclusions: Given the three length scales in any granular media: macroscopic, granular and microscopic, two temperatures: $T,T_g$ are relevant, and the entropy is the sum of all granular and microscopic degrees of freedom. Thermodynamics holds, and $T_g$ is a well-behaved, if one includes $T$ in all considerations. A jammed state at rest is in equilibrium, with the entropy being maximal. Fluctuation-dissipation theorem, correlating dissipation to thermal fluctuations, holds in granular media as in any other system. The strong, nonthermal grain-level stochasticity – such as force chains, or stick and slip motion – has yet to find a theory. But the macroscopic granular dynamics, averaged over thermal and grain-level fluctuations, is well accounted for by GSH.

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