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Elastic energy, fluctuations and temperature for granular materials

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Abstract. – We probe, using a model system, elastic and kinetic energies for sheared granular materials. For large enough P/E_y (pressure/Young’s modulus) and $P/\rho v^2$ (P /kinetic energy density) elastic dominates kinetic energy, and energy fluctuations become primarily elastic in nature. This regime has likely been reached in recent experiments. We consider a generalization of the granular temperature, T_g , with both kinetic and elastic terms and that changes smoothly from one regime to the other. This T_g is roughly consistent with a temperature adapted from equilibrium statistical mechanics.

We explore the role of elasticity in the energy and energy fluctuations of sheared dense granular systems. For dilated gas-like granular states, energy fluctuations are frequently described in terms of a temperature, defined as the fluctuating part of the kinetic energy, $T_k \equiv m\langle v^2 \rangle / 2$. Here, v is the local random component of the velocity. This definition is predicated on assumptions such as molecular chaos, absence of correlations, and short-lived collisions, that do not always apply. For dense systems of rigid particles, a very different concept, Edwards entropy, has been proposed [1]. This quantity is the logarithm of the number of jammed configurations consistent with all constraints on the system, and the Edwards temperature is $T_E^{-1} = \partial S_E / \partial V$, where V is the system volume.

Both of these pictures assume that minimal energy is stored in compressional modes of the particles. This assumption may be valid when the pressure is small compared to Young’s modulus, E_y . However, there are situations when this need not be the case. The main goal of this letter is to analyze via discrete element simulations (DES) the storage of energy and energy fluctuations for sheared dense granular material, taking account of elastic energy.

In order to better establish a context, we estimate the relative importance of kinetic and elastic energy for a simplified system. We imagine that spherical particles with a typical velocity, v , are subject to an applied force, L , at each contact. For simplicity, assume at first just a pair of opposing contacts, so that there is an effective pressure, $P = L/A$, where $A = \pi R^2$, and R is the radius of a sphere. The elastic energy per contact (assuming a Hertz-Mindlin contact law) is $\epsilon \propto L^{5/3}$. The ratio of elastic to kinetic energy for a particle with Young’s modulus E_y and density ρ is $R_E = \epsilon/K = C(P/E_y)^{2/3}(P/\rho v^2)$, where C is an $O(1)$ constant that depends on the Poisson ratio. On multiplying by the number of contacts per

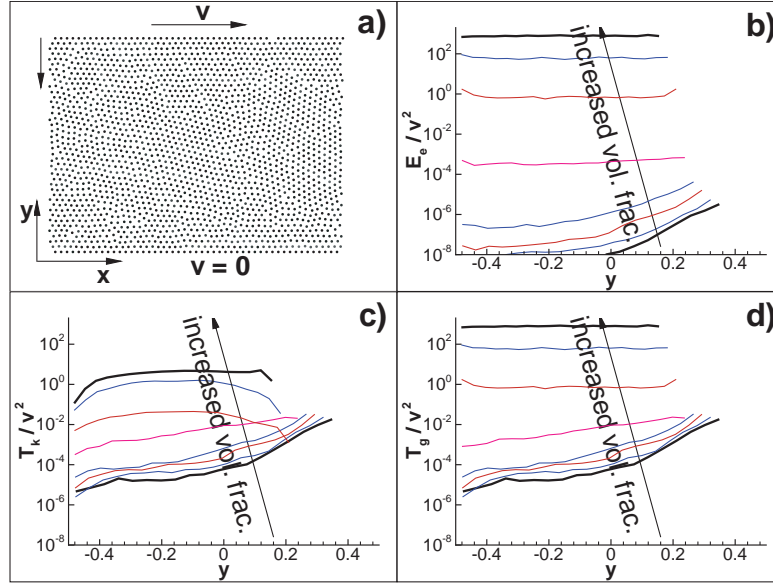


Fig. 1 – a) The geometry of the simulations (only centers of the particles are shown). b)-d) Elastic energy E_e , kinetic temperature T_k , and generalized temperature T_g (defined in the text) scaled by v^2 , as functions of the distance from the walls, y . The stationary wall is at $y = -0.5$, the shearing wall is to the right, and the shearing is in the out-of-plane direction ($v = 0.1$).

particle, it is possible to generalize this to a more realistic situation. When R_E is small, elastic energy is irrelevant, and *vice versa* when it is large, it should be included in a description.

We now consider R_E for two representative cases. For the experiments [2], $E_y = 5$ MPa, $P \sim 160$ Pa, and $\rho = 1.2$ g/cm³. Typical speeds range over 6×10^{-4} m/s $\leq v \leq 2 \times 10^{-2}$ m/s, so that $0.3 \leq R_E \leq 4 \times 10^2$. For glass spheres [3], E_y is larger by roughly a factor of 5000. Assuming densities $\rho \sim 2$ g/cm³, and pressures of $P \simeq 2000$ Pa corresponding to the base of a column 10 cm high in a gravitational field, $R_E \simeq 1$ for velocities of a few mm/s.

Hence, for slowly sheared dense granular systems, there exist velocity regimes for which elastic energy is the dominant mode of energy storage. In such a setting, neither T_k nor T_E is likely to provide a good measure of the random nature of the system.

In this context, we propose an extension of granular “temperature” that contains information on fluctuations of the elastic energy, and then compare this extension to a relation for temperature drawn from statistical mechanics. (A somewhat similar approach of applying equilibrium statistical theory has been taken in recent works on foams [4] and granular systems [5].) To carry out this exploration, we use DES of 2D particles that are subject to plane shear and (possibly) compression.

The generalization of “temperature” that we consider is based on the classical idea that for a lattice of elastic particles, the average fluctuating energy/particle is $3k_B T$. Using this as a heuristic guide, we define a generalized temperature that is $T_g = m\langle v^2 \rangle / 2 + k\langle x^2 \rangle / 2$, where v corresponds to the fluctuating part of the velocity, and x to the fluctuating part of the compression of a particle. Note that this definition provides a simple bridge between the extremes of a gas-like state and a highly compressed slowly evolving state.

In the simulation, particles are confined between two impenetrable straight parallel boundaries, as sketched in fig. 1a). The rough top boundary, which is 50 mean particle diameters

(d_m) long, moves at a steady speed, and induces shearing in the system. The boundary conditions in the shearing direction are periodic. This system avoids the nonuniformity that characterizes physical experiments, which typically exhibit shear bands [2]. Although we could have used the simpler Lees-Edwards conditions, we have concentrated on the present model so as to explore the influence of impenetrable boundaries, typical of physical experiments.

These simulations use a soft-disk/sphere model similar to what has been used in a number of granular simulations (see [6] and references therein). Here, we concentrate on two-dimensional polydisperse disks in a zero- g environment. The walls are made of identical particles that are rigidly attached. Forces between the particles have a normal component given by $\mathbf{F}_N = [k_f x - \gamma_N \bar{m}(\mathbf{v}_{i,j} \cdot \hat{\mathbf{n}})]\hat{\mathbf{n}}$, where k_f is a force constant, $r_{i,j} = |\mathbf{r}_{i,j}|$, $\mathbf{r}_{i,j} = \mathbf{r}_i - \mathbf{r}_j$, $\hat{\mathbf{n}} = \mathbf{r}_{i,j}/r_{i,j}$, $d = (d_i + d_j)/2$, $d_{i,j}$ are the diameters of the particles i and j , $x = d - r_{i,j}$ is the compression, $\mathbf{v}_{i,j} = \mathbf{v}_i - \mathbf{v}_j$, \bar{m} is the reduced mass, and γ_n is the damping constant related to the coefficient of restitution, e_n . The parameters represent photoelastic disks [2]; in particular, γ_n corresponds to $e_n = 0.5$. The tangential force is given by $\mathbf{F}_S = \text{sign}(-v_{\text{rel}}^t) \min(\gamma_s \bar{m} |v_{\text{rel}}^t|, \nu_k |\mathbf{F}_N^c|) \hat{\mathbf{s}}$, where v_{rel}^t is the relative velocity in the tangential direction $\hat{\mathbf{s}}$, $\gamma_s = \gamma_n/2$ and ν_k is the coefficient of friction between the particles. The equations of motion are then integrated using a 4th-order predictor-corrector method. Additional simulations (to be presented elsewhere) show that variation of the parameters or the force model modify only details of the results.

The simulations are performed with approximately 2000 polydisperse particles, with a radius variability of 10%. While polydispersity is important to avoid crystallization, the details of the size distribution are not: the results are very similar for different ranges of particle sizes, or a bidisperse distribution. Particles are initially placed on a lattice, given random velocities, and the system is then very slowly compressed to a desired volume fraction, ν . The results that follow use t , the time it takes the shearing wall to travel once across the domain of length $l = 50d_m$, as a time scale, and l/t as a velocity scale.

The quantities below are calculated using space-time averaging. Thus, the system is divided into cells, and averaged quantities are calculated for each cell. In particular, the kinetic temperature is defined by

$$T_k = \frac{1}{2} \left[\langle m(u')^2 \rangle + \langle m(v')^2 \rangle + \frac{\beta}{4} \langle m(d_p \omega')^2 \rangle \right],$$

where u, v are the components of particle velocity, d_p is the diameter of a particle, m is its mass ($m \sim d_p^2$), $\beta = 1/4$ for disks, and ω is the angular velocity. The primed averages are defined with zero mean, *e.g.*, $\langle u'v' \rangle = \langle uv \rangle - \langle u \rangle \langle v \rangle$.

The elastic energy is obtained by averaging *per collision*, not per particle. The difference between the two is significant for dense granular systems considered here, since particles typically experience multiple collisions (calculating elastic energy per particle greatly overestimates the elastic energy). If $x_{j,c}$ is the compression of particle j due to the collision c (two particles are assumed to participate in a collision if the distance between their centers is less than d), then our definition of the elastic energy in cell l is

$$E_{e,l} = \frac{1}{N_t n_l} \frac{k_f}{2} \sum_{k=1}^{N_t} \sum_{j=1}^{n_l} \sum_{c=1}^{n_{c,j}} [x_{j,c}]^2, \quad (1)$$

where n_l is the number of particles in cell l at a given time, and \bar{n}_l is the average number of particles during the period of $k = 1$ to $k = N_t \gg 1$ time steps (in practice, the averaging time scale is sufficiently short so that to a high degree of accuracy $n_l = \bar{n}_l$). Collisions may last over relatively long times, but even the fastest collisions are well resolved due to short

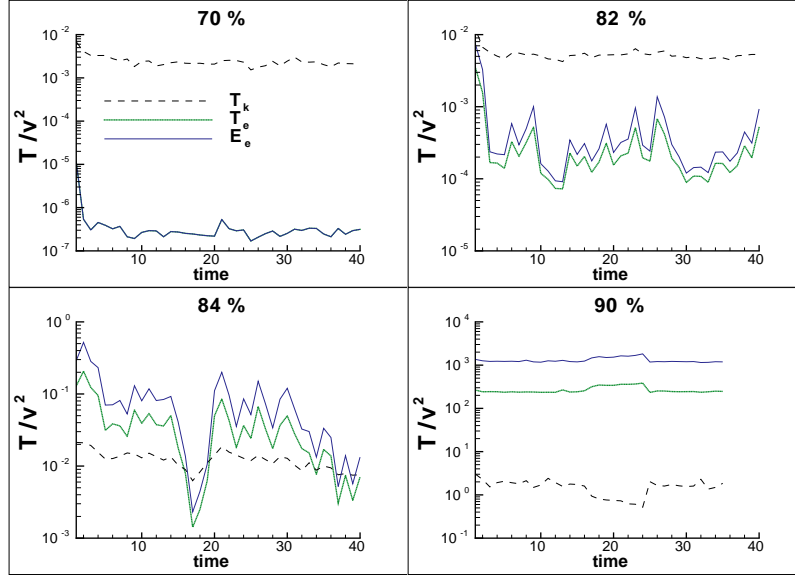


Fig. 2 – Elastic energy, kinetic and elastic temperatures for various ν 's, scaled by v^2 .

time step. Definition (1) ignores the energy used to overcome friction, and it clearly depends on the form of the normal force, *e.g.*, for a 3D systems, for which a Hertzian interaction law ($F_N \sim x^{3/2}$) is more appropriate, $E_{e,l}$ is of different form as well.

Figure 1b-c shows the elastic energy and kinetic temperature (scaled by the square of the shearing velocity v , and by the average mass of a particle) *vs.* the distance, y , from the shearing wall. For these simulations, ν is continuously increased by (slow) compression. ν increases from 65% (bottom) to 90% (top) (note that in 2D, random close packing and cubic close packing correspond to about 85% and $2\pi/\sqrt{3} \approx 90\%$, respectively). Clearly, as ν is increased, there is a transition region (about $\nu_c = 80\%$) where the energy stored in the internal degrees of freedom (elastic energy) becomes more relevant than the kinetic energy (see also fig. 2). The exact value of ν_c depends on the system parameters, in particular on the spring constant in our force model; here the spring constant is rather small since we simulate relatively soft particles. The y -dependence of the results is rather weak and becomes even weaker for higher ν 's. Hence, hereafter, we ignore the space dependence and use system averages (over all cells) of locally computed quantities.

As ν increases, the energy is mainly elastic, and T_k loses its relevance. In order to have a quantity that might play the same role as T_k in a dense granular system, we propose a generalized granular “temperature” by

$$T_g = T_k + T_e, \quad (2)$$

as a sum of T_k , and the “elastic” part T_e . T_e is defined as the variance of the *elastic* energy fluctuations about the mean, in a manner similar to T_k , which is the variance of *kinetic* energy fluctuations. This definition follows the classical statistical mechanics result where the mean fluctuations in the combined elastic and kinetic energy of an oscillator are proportional to the temperature. However, unlike this classical case, there is no reason to expect equipartition between elastic and kinetic modes. Rather, the ratio $T_e/(T_e + T_k)$ varies continuously from 0 in the dilute limit, to 1 in the dense limit.

The definition of T_e requires some care due to multiple collisions which a given particle may experience. One simple and natural definition that is consistent with the classical statistical definition of temperature for an oscillator is as follows. We first define the average elastic energy per particle in cell l as

$$\langle E_{e,l} \rangle = \frac{k_f}{2} n_c \langle x_l \rangle^2 = \frac{k_f}{2} n_c \left[\frac{1}{N_t \bar{n}_l n_c} \sum_{k=1}^{N_t} \sum_{j=1}^{n_l} \sum_{c=1}^{n_{c,j}} x_{j,c} \right]^2, \quad (3)$$

where $\langle x_l \rangle$ is the average compression per collision, and n_c is the average number of collisions per particle. Then,

$$T_{e,l} = \frac{k_f}{2} n_c \langle \delta x^2 \rangle = \frac{k_f}{2} n_c \langle (x_{j,c} - \langle x_l \rangle)^2 \rangle = E_{e,l} - \langle E_{e,l} \rangle, \quad (4)$$

where the last equality easily follows using eqs. (1) and (3). Figure 1d then shows the generalized temperature, T_g , defined by eq. (2). We clearly observe transition between the regime dominated by T_k for low ν , to that dominated by T_e for high ν . We note that in these simulations the y -dependence of T_e is very similar to the one of the elastic energy in fig. 1b).

Figure 2 shows T_k , T_e , and $\langle E_e \rangle$ vs. time, averaged over all cells, for four different ν 's. Unlike fig. 1, these results are obtained after shearing for long times at fixed ν 's. For higher ν 's, clearly $T_e \gg T_k$. Interestingly, there are rather large fluctuations of the results with ν just above $\nu_c \approx 80\%$, corresponding to the regime where elastic energy becomes predominant. Also, experiments have indicated a phase transition for comparable densities which may be related [2] (see also [7]). Generally, one might expect both glassy and/or jamming phenomena to dominate this regime, a point that we will explore elsewhere.

We further interpret T_g by comparing it to an alternative definition from equilibrium statistical mechanics. We consider, among various possibilities, a standard fluctuation-dissipation relation [8]:

$$\frac{dU}{dT} = \frac{\delta U^2}{T^2}, \quad (5)$$

which relates the (constant volume) heat capacity $c_v = dU/dT$ to the energy fluctuations. Here U is the total energy in the (usually conservative) system, T is the temperature, and $\delta U^2 = \langle U^2 \rangle - \langle U \rangle^2$. We use $U = E_{\text{kin}} + \langle E_e \rangle$, and ask whether T of eq. (5) and T_g are effectively equivalent: $T = T_g = T_k + T_e$. To check this idea, we now think of eq. (5) as a defining equation for $T_m = \sqrt{\delta U^2} / (dU/dT_g)$ (here T_m stands for ‘‘model temperature’’). The degree of agreement between T_m and T_g will provide some indication of the utility of the definition for T_g . Note that we should not expect perfect or possibly even any agreement, since we are considering a strongly dissipative system far from equilibrium.

Figure 3 shows typical data used to determine c_v , which is needed for calculating T_m . The range of U 's shown in fig. 3 corresponds to $0.0001 < v < 40$. For $\nu = 80\%$, $U \sim T_g$ over almost 10 decades. For $\nu = 86\%$, $U \sim T_g^a$, where $a \simeq 2.0$. However, in this case, there is a deviation from the power law fit for slow shearing, and we are limited to a smaller range of U 's, since most of the energy is stored in the system as elastic energy. In order to obtain better data for $U(T_g)$ for slow shearing at higher densities, we determine both U and T_g as functions of v , see fig. 3b). We then find to a good approximation that both U and T_g are proportional to $\ln(v)$. This logarithmic dependence for slow shearing is, to the best of our knowledge, the first computational confirmation of recent experimental results [9], and will be presented in more detail elsewhere. For our purposes here, it is sufficient to extract $U(T_g)$.

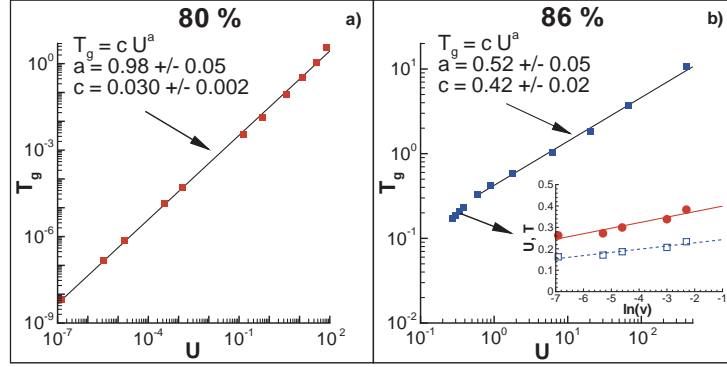


Fig. 3 – Generalized temperature *vs.* average energy for two different ν 's (increased U corresponds to increased shearing velocity v). The lines are the least-square fits to the data. In the inset of b), U (solid line, filled circles) and T_g (broken line, squares) are plotted *vs.* $\ln(v)$ for slow shearing.

The dependence of $U(T_g)$ is interesting. We note that $U \sim T_g$ for $\nu = 80\%$ is similar to a recent simulation of sheared foams [4]. However, the result $U \sim T_g^2$ for $\nu = 86\%$ and for not too slow shearing, see fig. 3b), is striking and deserves some comment. Although it may appear that the role of elastic energy is crucial for this change of the exponent a , this does not seem to be the whole story. As shown in fig. 4, even for this high ν , E_k is still dominant for high enough shearing rates. Despite this, a is still different compared to the one for lower ν 's. An interpretation is that large ν leads to decreased mobility, bringing the system closer to jamming, and limits the growth of T_g with U . However, for non-rigid particles, complete jamming is avoided. We note that in additional simulations (not shown) we observe that the change of the exponent a from 1 to 2 occurs in a very narrow range of volume fractions, centered at about 84% (the exact location depends on the shearing velocity). We do not observe any meaningful change of a as the volume fraction is increased beyond 86%.

Figure 4 contains a summary of the various types of temperatures for two ν 's. As already noted, for $\nu = 80\%$, most of the energy is still kinetic, while for $\nu = 86\%$, elastic energy

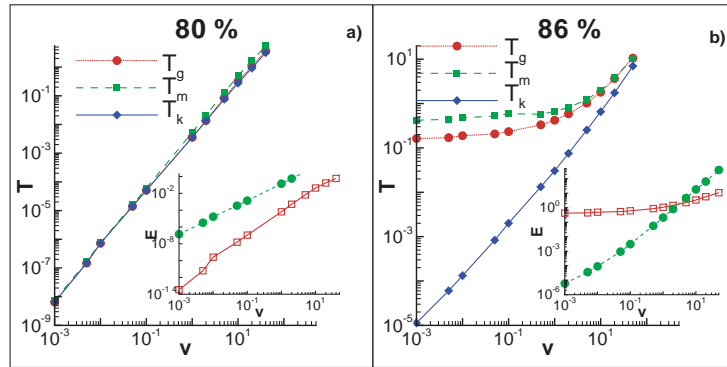


Fig. 4 – Generalized, kinetic, and “model” temperature (see the text and eq. (5)) for two volume fractions. Error bars are approximately represented by the size of the symbols. The insets show kinetic energy (filled circles) and average elastic energy (squares). In a), $T_k = T_g$, up to the resolution of the plot.

is essential. For $\nu = 80\%$, T_k is dominant (it is indistinguishable from T_g in fig. 4a), and also it satisfies the model (5) since $T_k \approx T_m$). However, for $\nu = 86\%$ and for slow shearing, T_k is smaller by 4 orders of magnitude than T_g and T_m ! Thus, T_k cannot be used to even approximately describe a dense slowly sheared granular system. This difference decreases for higher shearing rates, but only at very high shearing is there good agreement. We note that the results presented here apply to any confined, sheared, granular system.

We now discuss, in the context of fig. 4, the degree of agreement between T_g and T_m . While the agreement is not perfect, these two quantities are qualitatively similar. Therefore, these studies already demonstrate the clear need to incorporate elastic energy and elastic fluctuations, and that T_g has utility as a generalized granular temperature. We note that preliminary results (to be discussed elsewhere) show that a similar agreement can be found using a Hertzian interaction law.

Clearly, there remain many open questions regarding the extent to which the various temperatures serve similar functions to their molecular counterpart. Here we only note that at least qualitatively one can show that these temperatures can be used in the context of thermal conduction, *i.e.* that there is a flow of heat from hot to cold regions. We also note that the distributions of both kinetic and elastic energy are strongly non-Gaussian for a significant range of the parameters analyzed here. These energy distributions, as well as other features related to the proposed temperature generalization, will be analyzed in future works. One of these features which is of particular interest is to relate T_g to the time-dependent temperatures that have been discussed in the context of glasses, colloids, and granular materials [10–12].

This work clearly demonstrates a regime of pressures and speeds for which elastic energy and elastic energy fluctuations are an essential part of the dynamics for slow shearing. We view this as a first step towards a generalized “thermal” description for the dense granular systems where the kinetic contribution to the energy does not suffice. The ultimate test will be to perform physical experiments where the validity of the proposed concepts can be verified.

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