Elastic Energy, Fluctuations and Temperature for Granular Materials

Lou Kondic\(^{(1)}\) and R. P. Behringer\(^{(2)}\)

\(^{(1)}\)Department of Mathematical Sciences & Center for Applied Mathematics & Statistics
New Jersey Institute of Technology, Newark, NJ 07102

\(^{(2)}\)Department of Physics & Center for Nonlinear and Complex Systems
Duke University, Durham NC, 27708-0305

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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 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.

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Lees-Edwards conditions, we have concentrated on the present model so as to explore the influence of boundaries, typically present in physical experiments.

These simulations closely follow the soft-disk/sphere model to describe various granular systems (see the 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 \( \mathbf{F}_N = [k_f x - \gamma_N \mathbf{n} (\mathbf{v}_{i,j} \cdot \mathbf{n})] \) where \( k_f \) is a force constant, \( r_{i,j} = |\mathbf{r}_{i,j}| \), \( \mathbf{n} = \mathbf{r}_{i,j}/r_{i,j} \), \( d = (d_i + d_j)/2 \), \( d_{i,j} \) are the diameters of the particles \( i \) and \( j \), \( x = d - r_{i,j} \) is the compression, \( \mathbf{v}_{i,j} = \mathbf{v}_i - \mathbf{v}_j \), \( \mathbf{m} \) is the reduced mass, and \( \gamma_n \) is the damping constant related to the coefficient of restitution, \( e_n \).

The parameters represent photoelastic disks in particular, \( \gamma_n \) corresponds to \( e_n = 0.5 \). The tangential force is given by \( \mathbf{F}_S = \text{sign}(-v_{rel}^t) \min (\gamma_s m |v_{rel}^t|, \mu_k |\mathbf{F}_N^t|) \mathbf{s} \) where \( v_{rel}^t \) is the relative velocity in the tangential direction \( \mathbf{s} \), \( \gamma_s = \gamma_n/2 \) and \( \mu_k \) 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, \( \nu \). The results that follow use \( t \), the time it takes the shearing wall to travel once across the domain, as a time scale, and \( l/t (l = 50d_m) \) 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

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

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 \( \omega \) is the angular velocity. The primed averages are defined with zero mean, e.g., \( \langle u v' \rangle = \langle u \rangle \langle v \rangle' \).

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. If \( x_{j,c} \) is the compression of particle \( j \) due to the collision \( c \), then our definition of the elastic energy in cell \( l \) is

\[
E_{e,l} = \frac{1}{N_l n_l} \frac{k_f}{2} \sum_{k=1}^{N_c} \sum_{j=1}^{n_c} \sum_{c=1}^{n_{c,j}} [x_{j,c}]^2,
\]

where \( n_l \) is the number of particles in cell \( l \) at a given time, and \( n_l \) is the average number of particles during the period of \( N_l \approx 1 \) time steps (in practice, the averaging time scale is sufficiently short so that to a high degree of accuracy \( n_l = \bar{n}_l \)).

Definition ignores the energy used to overcome friction, and its form 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.

The elastic energy and kinetic temperature are obtained by averaging of the shearing velocity \( \nu \), and by the average mass of a particle vs. distance, \( y \), from the shearing wall. For these simulations, \( \nu \) is continuously increased by (slow) compression. \( \nu \) 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 \( \nu \) 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. 4). The \( y \)-dependence of the results is rather weak and becomes even weaker for higher \( \nu \)’s. Hence, hereafter, we ignore the \( y \)-dependence and use system averages of locally computed quantities.

As \( \nu \) 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

$$T_g = T_k + T_e, \tag{2}$$

as a sum of $T_k$, and the 'elastic' part $T_e$. $T_e$ is defined as
the mean fluctuation of elastic energy, in a manner similar to $T_k$, which is the mean fluctuation of kinetic energy. 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 from 0 in the dilute limit, to 1 in the dense limit.

The definition of $T_e$ requires some care due to multiple collisions. 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

$$\langle E_{e,l} \rangle = \frac{k_f}{2} n_e \langle x_i \rangle^2 = \frac{k_f}{2} n_e \left[ \frac{1}{N_l n_l n_c} \sum_{k=1}^{N_l} \sum_{j=1}^{n_l} \sum_{l=1}^{n_c} x_{j,c} \right]^2, \tag{3}$$

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

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

where the last equality easily follows using (1) and (3).

Figure 2 shows $T_k$, $T_e$, and $\langle E_e \rangle$ vs. time, for four different $\nu$'s. Unlike the results of Fig. 1 these results are obtained after shearing for long times at fixed $\nu$'s. For higher $\nu$'s, clearly $T_e \gg T_k$. Interestingly, there are rather large fluctuations of the results with $\nu$ 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 to (see also [3]). 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 statistical mechanics. We consider, among various possibilities, the standard relation

$$\frac{dU}{dT} = \frac{\delta U^2}{T^2}, \tag{5}$$

dissipative system far from equilibrium. We emphasize that there are no fitting parameters and that the results that follow are obtained directly from simulations.

![Figure 2: Elastic energy, kinetic and elastic temperatures for various $\nu$'s, scaled by $\nu^2$.](image)

![Figure 3: Generalized temperature versus average energy for two different $\nu$'s (increased $U$ corresponds to increased shear velocity $v$). The lines are the least square fits to the data.](image)
FIG. 4: Generalized, kinetic, and ‘model’ temperature (see the text and Eq. 5) for two volume fractions. Error bars (resulting from statistical uncertainty of the results, as well as from the uncertainty introduced by the least square fits from Fig. 3) are approximately represented by the size of the symbols. The insets show kinetic energy (filled circles) and average elastic energy (squares).

Figure 3 shows typical data used to determine $c_v = dU/dT_g$ needed for $T_m$. The range of $U$’s shown in Fig. 4 corresponds to $0.0001 < v < 40$. For $v = 80\%$, $U \sim T_g$ over almost 10 decades. For $v = 86\%$, $U \sim T_g^2$, where $a \approx 2.0$. 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 $U$ and $T_g$ as functions of $v$, see Fig. 4b. 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 [6], and will be presented in more detail elsewhere. For our purposes here, it is sufficient to extract $U(T_g)$.

The dependence of $U(T_g)$ is interesting. We note that $U \sim T_g$ for $v = 80\%$ is similar to a recent simulation of sheared foams [7]. However, the result $U \sim T_g^2$ for $v = 86\%$ and for not too slow shearing ($U > 1$, see Fig. 4b) is striking and deserves some comment. Although the increased role of elastic energy is important here, this does not appear to be the whole story, as seen in the context of Fig. 4. Here, we show that even for this high $v$, for fast enough shearing the kinetic energy is still dominant. Our preliminary interpretation is that increased volume fraction contributes significantly to decreased mobility (jamming) of the granular system, therefore reducing the increase of $T_g$ with $U$.

Figure 4 contains a summary of the various types of temperatures considered in this study for two $v$’s. As already noted, for $v = 80\%$, most of the energy is still kinetic, while for $v = 86\%$, elastic energy is essential. For $v = 80\%$, $T_k$ is dominant, and also it satisfies the model [3] since $T_k \approx T_m$. However, for $v = 86\%$ 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.

The agreement between $T_g$ and $T_m$ is not perfect, although prefect agreement is not to be expected. These studies demonstrate the clear need to incorporate elastic energy and elastic fluctuations, and that $T_g$ has utility as a generalized granular temperature. Nevertheless, there remain many open questions regarding the extent to which the various temperatures serve similar functions to their molecular counterpart. We will present detailed results addressing this type of question elsewhere. Here we note that at least qualitatively one can show that these temperatures can be used in the context of thermal conduction, i.e. the 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.

There are other possible tests of the proposed generalization, as recently discussed on the context of sheared foams [6]. The ultimate test will be to perform physical experiments where the validity of the proposed concepts can be verified. In the theoretical direction, it will be of interest to relate the generalized granular temperature proposed here to the one resulting from Edwards-entropy based approach.

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