Elastic Energy, Fluctuations and Temperature for Granular Materials

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Elastic Energy, Fluctuations and Temperature for Granular Materials

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In our recent work (Europhys. Lett. **67**, 205 (2004)) we have shown that in granular systems characterized by large volume fractions, the elastic energy dominates the kinetic energy, and energy fluctuations are primarily elastic in nature. As a logical consequence of this observation, we have started exploring possible generalizations of the concept of granular temperature to dense, jammed systems where kinetic granular temperature is not expected to be relevant, at least from the energetic point of view. Therefore, we have introduced generalized granular temperature, which turns out to be roughly consistent with a temperature based on the equilibrium statistical mechanics. In this paper, we discuss the influence of various system properties on this new generalized granular temperature. These properties include the shearing rate, as well as the material properties such as stiffness, elasticity and friction.

1 INTRODUCTION

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, $T_k \equiv m < v^2 > /2$. 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 (Edwards 1994). 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.

Neither of these pictures explicitly includes the energy stored in compressional modes of the particles. This approach may be valid when the pressure is small compared to the Young's modulus, E_y. However, there are numerous situations when this is not the case. Some of these are discussed in our earlier work (Kondic and Behringer 2004), where we present one approach towards inclusion of elastic energy and energy fluctuations in the statistical description of granular systems. In this paper, we discuss further the concept of temperature appropriate for dense granular systems, and also present new computational results that illustrate how material and systems properties influence the energy balance and energy fluctuations.

The crucial point on which we concentrate is the fact that for any sheared dense granular systems, there exist velocity regimes for which elastic energy is the dominant mode of energy storage. In such a setting, neither kinetic granular temperature, 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. 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 $3k_BT$. Using this as a heuristic guide, we define a generalized temperature that is $T_g = m < v^2 > /2 + k < x^2 > /2$, where x corresponds 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.

2 DESCRIPTION OF THE SYSTEM

A description of the simulational system is given in more detail in (Kondic and Behringer 2004); here we outline the main features. Figure 1 shows a sketch of the flow geometry. Circular, frictional, inelastic particles are confined between two rough impenetrable straight parallel boundaries. The top boundary, which is 50 mean particle diameters (d_m) long, moves at a steady speed, and induces shear; the boundary conditions in the shearing direction are periodic.

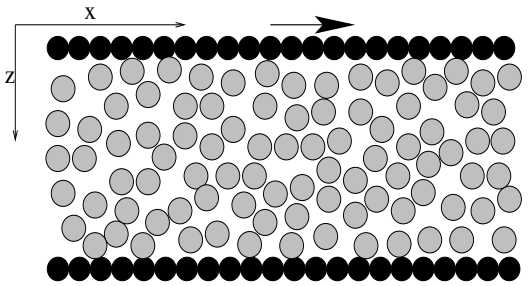


Figure 1: Sketch of the flow geometry. The upper wall imposes shear on the system by moving with constant velocity, V in the $+x$ direction, and also controls the volume fraction by quasistatic compression imposed by motion of the upper wall in the $+z$ direction.

The simulations use a soft-disk/sphere model similar to what has been used in a number of granular simulations (see (Kondic 1999) and references therein). Here, we use 2D 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

$$\mathbf{F}_N = \left[k_f x - \gamma_N \bar{m}(\mathbf{v}_{i,j}\cdot\hat{\mathbf{n}})\right], \qquad (1)$$

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 tangential force is given by

$$\mathbf{F}_S = sign(-v^t_{rel})min\left(\gamma_s\bar{m}|v^t_{rel}|, \mu_k|\mathbf{F}^c_N|\right)\hat{\mathbf{s}}, \qquad (2)$$

where v^t_{rel} is the relative velocity in the tangential direction $\hat{\mathbf{s}}$, $\gamma_s = \gamma_n/2$ and μ_k is the coefficient of friction between the particles. The equations of motion are then integrated using a 4th order predictor-corrector method. The simulations are performed with approximately 2000 polydisperse particles, with a radius variability of 10%; very similar results to the ones presented here have been also obtained with different polydispersity ratios, or with bidisperse particles. 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. If not specified differently, we use a shearing velocity $V = 1$, the spring constant is $k_n = 4\cdot 10^3$ mg/d_m (m is a particle mass and g is acceleration of gravity), the coefficient of restitution $e_n = 0.5$, and the coefficient of tangential friction is $\mu_k = 0.5$. The choice of the parameters is motivated by experiments performed using relatively soft frictional photoelastic discs (Howell et al. 1999).

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 cell-averaged 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

$$E_{e,l} = \frac{1}{N_t n_l}\frac{k_f}{2}\sum_{k=1}^{N_t}\sum_{j=1}^{n_l}\sum_{c=1}^{n_{c,j}}\left[x_{j,c}\right]^2, \qquad (3)$$

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.

We have performed two types of simulations: one where ν is very slowly increased (by moving the upper wall in the z direction– system properties are calculated while the systems is being compressed) and the one in which the volume fraction is kept fixed and the system variables are calculated over long periods of time. In (Kondic and Behringer 2004) we mostly concentrate on the results of these latter simulations, therefore analyzing a discrete set of ν's. However, additional simulations have shown that there is no observable difference between results obtained in the continuously compressed systems and those characterized by constant ν, as long as the compression is slow. Here we concentrate on these continuously compressed case,thus analyzing directly how changes of ν influence the results.

3 RESULTS

Figure 2 shows the results for temperatures and energies averaged over the whole system (spatial dependence is discussed in more detail elsewhere). Here, ν is continuously increased from 65% to 92% (note that in 2D, random close packing corresponds to about 85%). The most prominent feature visible in this figure is the sharp increase of the elastic energy (thick solid line) as the volume fraction is increased. At some critical volume fraction, ν_c (close to 82% for the parameters as used in Fig. 2) the dominant energy contribution changes from kinetic to elastic. The exact value of ν_c depends on the system parameters, as we will see below.

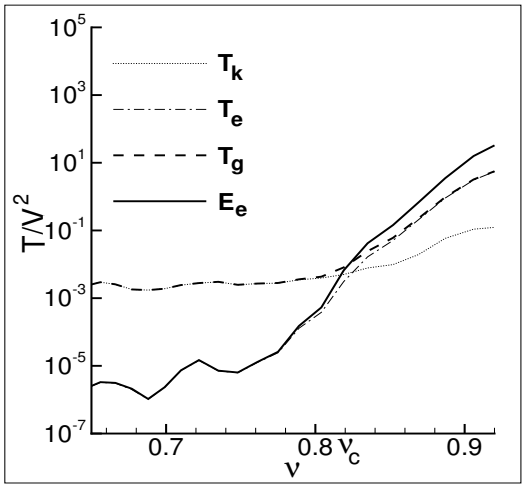


Figure 2: Temperatures and energies averaged over the whole computational domain as a function of continuously changing volume fraction. Note that the generalized temperature, T_g (see Eq. 4), provides a smooth connection between kinetic-dominated and elastic-dominated regimes. Here, ν_c is the volume fraction for which T_k and T_e are approximately equal; $V = 1$, $\mu_k = 0.5$, $k_n = 4.0 \cdot 10^3$, and $e_n = 0.5$.

In (Kondic and Behringer 2004) we show that the behavior close to this transition is characterized by large energy fluctuations; we also note that ν_c is close to the volume fraction at which a second-order phase transition has been observed experimentally, in annular Couette cell (Howell et al. 1999).

As ν increases, the energy is mainly elastic, and T_k loses its relevance (Fig. 2). In order to have a quantity for a dense system that might be comparable to T_k, we formulate a generalized temperature:

$$T_g = T_k + T_e, \tag{4}$$

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 parallel to T_k, which is the variance of *kinetic* energy fluctuations. This definition follows the classical statistical mechanics: the variance of combined elastic and kinetic energy of an oscillator yields the temperature. 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 uses the average elastic energy per particle in cell l

$$\langle E_{e,l} \rangle = \frac{k_f}{2} n_c \langle x_l \rangle^2 = \frac{k_f}{2} n_c \left[\frac{1}{N_t \bar{n}_l n_c} \sum_{k=1}^{N_t} \sum_{j=1}^{n_l} \sum_{c=1}^{n_{c,j}} x_{j,c} \right]^2 , \tag{5}$$

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

$$T_{e,l} = \frac{k_f}{2} n_c \langle \delta x^2 \rangle = \frac{k_f}{2} n_c \langle (x_{j,c} - \langle x_l \rangle)^2 \rangle = E_{e,l} - \langle E_{e,l} \rangle , \tag{6}$$

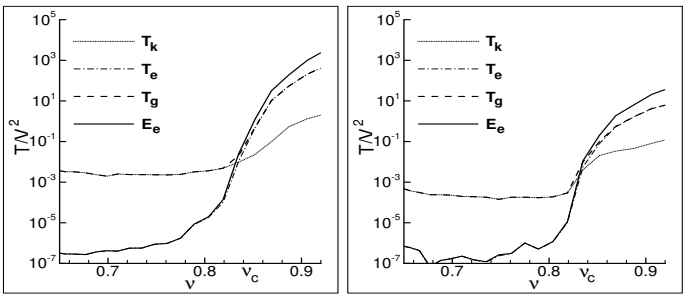
where the last equality is based on Eqs. 3 and 5. T_g, defined by Eq. 4 is also shown in Fig. 2. Clearly there is a transition from the T_k-dominated regime for low ν, to one dominated by T_e for high ν. The difference between E_e and T_e in Fig. 2 measures the average elastic energy in the system; $< E_e >$ becomes significant only for rather large ν's.

In (Kondic and Behringer 2004) we outlined the relation of the newly introduced concept of generalized granular temperature to the one that may be derived using equilibrium statistical mechanics. (A somewhat similar approach of applying equilibrium statistical theory has been taken in recent works on foams (Ono et al. 2002) and granular systems (Makse and Kurchan 2002).) We note that there are interesting questions regarding time dependence of granular temperatures and energies (O'Hern et al. 2004). We do not consider these issues here, but instead concentrate in more detail on the influence which material properties, as well as shearing velocity, have on the transition between kinetic-dominated and elastic-dominated regimes.

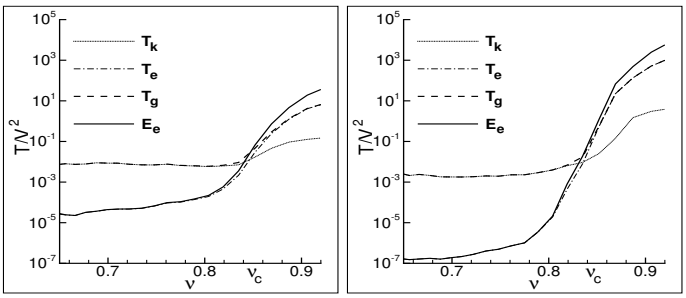
3.1 *Parametric Dependence*

There many parameters that may influence the systems response to the imposed shear. Here we concentrate on the material properties: elasticity, friction, stiffness, and on the shearing velocity, V. It should be noted that the V's that we use here are in the regime that produce linear or approximately linear velocity profiles. Therefore, we do not consider the regime of fast shear, where the shearing velocity is comparable to the speed of the shear waves in the system, which may lead to nonlinear velocity profiles and possibly to different system response (Xu et al. 2005).

In Fig. 3 and the following, we discuss the effect of several parameters. We note that for all cases, there is continuous, monotonic change for each parameter.



(a) $V = 0.1$. (b) $\mu_k = 0.1$.



(c) $e_n = 0.9$. (d) $k_f = 1.024 \cdot 10^6$.

Figure 3: Parametric dependence of various temperatures and energies. The parameters that are not specified are the same as in Fig. 2.

Shearing velocity. A decrease of V (Fig. 3(a) vs. Fig. 2) leads to a slight increase of ν_c where elastic energies dominate kinetic. While changing V has very weak effect on T/V^2 for small ν's (as expected, the system temperatures and energies scale with V^2), for large ν's, E_e and T_e do not scale with V^2. This can be explained by the onset of jamming.

Friction. From Fig. 3(b), smaller μ_k's shift the transition point to higher ν's and lead to faster growth of E_e as ν is increased. This may occur because for small ν's, low friction leads to decreased particle mobility, since friction enhances momentum transfer between the particles (for this reason, for small ν's, T_k increases as μ_k is increased). E_e is also smaller for smaller μ_k since the dynamics are slower, leading to a lower collision rate. However, as ν increases, E_e and T_e are not strongly influenced by μ_k, and the transition to the elastic dominated regime is faster.

The restitution coefficient e_n (Fig. 3(c)) influences the transition rather weekly. The main effect is that for larger e_n, both kinetic and elastic temperatures and energies are higher for small ν's.

Stiffness. We specified earlier that the results of this paper mostly concentrate on relatively soft particles, e.g. the force constant k_f is relatively small (recall also that Young modulus, $E_y \propto \sqrt{k_f}$). We performed simulations with a number of much larger values for k_f and found that its influence was relevant only for large ν's. This is illustrated in Fig. 3(d), where we observe much larger values of E_e and T_e for stiff particles, but almost no change for small ν's. The transition point ν_c is slightly shifted towards larger ν's, but there is only a qualitative change in the data for T/V^2, even in this case of much stiffer particles.

Clearly, there remain many open questions regarding the extent to which various temperatures serve similar functions to their molecular counterpart. These include issues such as heat conduction, time-dependence, among others. In this work, we have concentrated on demonstrating the fact that the transition between the kinetic-dominated and elastic-dominated regimes is a robust phenomenon whose main features are preserved for a wide range of material properties, such as stiffness, restitution coefficient, or friction. Therefore, it is a generic feature of granular systems that deserves to be further explored.

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