LECTURE 2 - Statistical Ensembles for Jammed Granular States

Notes based on Henkes, O'Hern and Chakrabory, PRL 99, 038002 (2007), Henkes and Chakraborty , PRE 79, 061301 (2009), and Henkes, PhD thesis, Brandeis

Equilibrium - microcanonical to canonical

We quickly review the steps one takes in ordinary equilibrium statistical mechanics, in going from the microcanonical to the canonical ensemble.

In the microcanonical ensemble, energy is *conserved*. One *assumes* that all states with the same total energy E are *equally likely*, and computes microcanonical averages by averaging observables over all states with the same E, using equal weights. For N particles in a box of volume V, one counts the number number of states $\Omega(E, V, N)$ with total energy E. The temperature is *defined* by $1/T = \partial S/\partial E$, with $S(E) = \ln \Omega(E)$ the entropy.

Consider now a small subsystem with N particles in volume V, and the subsystem is in contact with a big reservoir with which it can exchange energy. The reservoir contains $N_R \gg N$ particles in a volume $V_R \gg V$. The total system of subsystem + reservoir is treated in the microcanonical ensemble. Since energy is *additive*, the total energy $E_T = E + E_R$ is fixed. One *assumes* the subsystem and the reservoir are uncorrelated and so the number of states of the total system factorizes,

$$\Omega_T(E_T) = \sum_E \Omega(E)\Omega_R(E_T - E)$$

One then expands for $E \ll E_T$,

$$\Omega_R(E_T - E) = \exp\{\ln \Omega_R(E_T) - [\partial \ln \Omega_R/\partial E_T]E\} \sim \exp\{-E/T_R\}$$

In equilibrium we know that the temperatures of the subsystem and reservoir equilibrate, $T = T_R$, and so if we assume that the probability to find the subsystem with energy E is proportional to the number of states in which the subsystem has energy E and the reservoir has $E_T - E$, then we get the canonical distribution,

$$P(E) \sim \Omega(E) \exp\{-E/T\}$$

Edwards volume ensemble for granular matter

Consider a jammed granular system of N rigid, incompressible, particles confined to a box of volume V. At a fixed packing fraction ϕ, there will in general be many possible distinct jammed states. Because the granular system is at $T = 0$, it will not on its own explore its phase space of allowed states unless it is physically perturbed (stirred, vibrated, sheared, etc.). Experiments on vibrated granular systems suggest that such systems do obey reproducible behavior, i.e. if vibrated with some frequency and amplitude, then allowed to relax, the system explores a well defined reproducible set of states.

To develop a statistical mechanics for such granular material, Edwards borrowed the above ideas from equilibrium, but now applying the arguments to the system *free volume* as the conserved quantity that takes the place of energy. He noted that for rigid particles the total free volume is obviously conserved, and that it is additive over subsystems. If $\Omega(V, N)$ is the number of distinct mechanically stable states of N particles in a box of volume V, Edwards defined the *compactivity* $X(V)$ by

$$1/X = \partial \ln \Omega / \partial V$$

Asserting that all mechanically stable states are equally likely, the above thus defines the microcanonical volume ensemble for granular materials.

Consider now a small subsystem in contact with the reservoir consisting of the large rest of the system. Since free volume is additive and conserved, if one makes the assumption that the number of states factorizes as the product of number of states of the subsystem times the number of states of the reservoir, one can complete the steps to the canonical ensemble and argue that the probability that some small subsystem of the granular material will be in a state ν with free volume v_ν is given by

$$P_\nu \sim \exp\{-v_\nu / X\}$$

The validity of Edwards' assumption, that all mechanically stable states with the same free volume are equally likely, remains in controversy. In the absence of more information, however, it is not clear what else to try! It is used in the same spirit as a *maximum entropy* principle - if one has a complex system, and knows only the average value of certain observables, one assumes that the probability distribution p_ν for possible configurations ν is the one that maximizes the entropy $S = -\sum_\nu p_\nu \ln p_\nu$ subject to the constraints of what average values are known. The resulting distribution has the same canonical ensemble form as above, with the Lagrange multiplier that enforces the constraint of the known average quantity playing the role of an inverse temperature. Whether this assumption is valid or not is something to be tested experimentally (or numerically) in different physical situations.

The Edwards ensemble is best applied to rigid frictional particles. If particles are not rigid, but can deform and press into each other, then free volume is not strictly conserved. If particles are rigid but frictionless, the only mechanically stable states occur at the single packing fraction ϕ_J described by $X = 0$. Only for frictional rigid particles can mechanically stable states be found over a range of packing fractions ϕ and one can have finite values of compactivity X (see Nature paper by Makse cited in Lecture 1).

Stress ensemble

To describe an ensemble for frictionless deformable (soft core) particles one needs a different conserved quantity to take the place of free volume. One candidate is the total force moment tensor, which we now consider.

We consider the simplest case of frictionless spheres interacting with a pairwise soft core potential, $V_{ij}(r_{ij})$, when they touch (i.e. $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i| < R_i + R_j$), and zero otherwise. We allow for polydisperse spheres with differing radii R_i.

The interaction energy is then

$$U = \frac{1}{2}\sum_{i,j} V_{ij}(r_{ij})$$

and the stress (or pressure) tensor is given by

$$\hat{\sigma} = \frac{1}{2V}\sum_{i,j} \mathbf{r}_{ij}\mathbf{F}_{ij}$$

with $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ the separation from particle i to particle j, and $\mathbf{F}_{ij}$ the contact force from particle i acting on particle j. If α and β denote spatial components, then

$$\hat{\sigma}_{\alpha\beta} = \sigma \quad \text{the shear stress, and} \quad \hat{\sigma}_{\alpha\alpha} = p \quad \text{the pressure}$$

Also

$$p = \frac{1}{d}\text{trace}\,\hat{\sigma} = \frac{1}{d}\frac{1}{2V}\sum_{i,j} \mathbf{r}_{ij}\cdot\mathbf{F}_{ij} = \frac{1}{2V}\sum_{i,j} r_{ij}F_{ij}$$

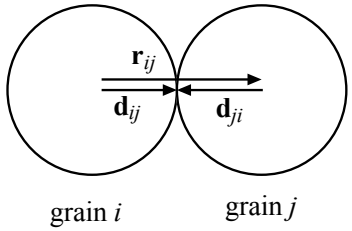
where d is the dimension of the system and the last equality follows since, for spherical particles, the contact force is always in the radial direction.

Consider now the total force moment tensor defined by

$$\hat{\mathbf{\Sigma}} = V\hat{\sigma} = \frac{1}{2}\sum_{ij} \mathbf{r}_{ij}\mathbf{F}_{ij}$$

We will show that $\hat{\mathbf{\Sigma}}$ is a conserved quantity - if one fixes the boundary of the system, then no local rearrangements of interior particles can change the value of $\hat{\mathbf{\Sigma}}$. We will also show that $\hat{\mathbf{\Sigma}}$ is additive over subsystems. Thus $\hat{\mathbf{\Sigma}}$ obeys the two essential conditions needed to create a statistical ensemble.

Denote $\mathbf{d}_{ij}$ as the displacement from the center of particle i to the point of contact with particle j. One then has $\mathbf{r}_{ij} = \mathbf{d}_{ij} - \mathbf{d}_{ji}$



Then, using $\mathbf{F}_{ij} = -\mathbf{F}_{ji}$ we have,

$$\hat{\mathbf{\Sigma}} = \frac{1}{2}\sum_{ij} \mathbf{r}_{ij}\mathbf{F}_{ij} = \frac{1}{2}\sum_{ij} (\mathbf{d}_{ij} - \mathbf{d}_{ji})\mathbf{F}_{ij} = \frac{1}{2}\sum_{ij} (\mathbf{d}_{ij}\mathbf{F}_{ij} + \mathbf{d}_{ji}\mathbf{F}_{ji}) = \sum_{ij} \mathbf{d}_{ij}\mathbf{F}_{ij} = \sum_{i} \hat{\sigma}_i$$

where

$$\hat{\sigma}_i = \sum_{j}{}' \mathbf{d}_{ij}\mathbf{F}_{ij}$$

is the microscopic stress tensor for particle i (here the sum is over all particles j in contact with i).

One can then define the stress tensor for a connected volume V as

$$\hat{\mathbf{\Sigma}}_V = \sum_{i \in AV} \hat{\sigma}_{\mathbf{i}}$$

We now show that $\hat{\mathbf{\Sigma}}_V$ only depends on the boundary of V (Ball and Blumenfeld, PRL 88, 115505 (2002)). The calculation is simplest in 2D, where we will now call the volume A, the area. Consider a cluster of neighboring grains as shown below, where i, j, k, l, m label grains, and ν, μ, λ, τ label the voids surrounding grain i.

One can define height variables $\mathbf{h}$ that sit on the centers of each void, as follows. Define the height on void ν as $\mathbf{h}_{i\nu} \equiv \mathbf{h}_0$, an arbitrary constant vector. Then define

$$\mathbf{h}_{i\mu} - \mathbf{h}_{i\nu} = -\mathbf{F}_{ij}$$

where μ is the void progressing counterclockwise from void ν, and $\mathbf{F}_{ij}$ is the contact force at the contact that separates voids ν and μ. Thus

$$\mathbf{h}_{i\mu} = \mathbf{h}_{i\nu} - \mathbf{F}_{ij} = \mathbf{h}_0 - \mathbf{F}_{ij}$$

Proceeding similarly,

$$\mathbf{h}_{i\lambda} = \mathbf{h}_{i\mu} - \mathbf{F}_{ik} = \mathbf{h}_0 - \mathbf{F}_{ij} - \mathbf{F}_{ik}$$

$$\mathbf{h}_{i\tau} = \mathbf{h}_{i\lambda} - \mathbf{F}_{il} = \mathbf{h}_0 - \mathbf{F}_{ij} - \mathbf{F}_{ik} - \mathbf{F}_{il}$$

$$\mathbf{h}_{i\nu} = \mathbf{h}_{i\tau} - \mathbf{F}_{im} = \mathbf{h}_0 - \mathbf{F}_{ij} - \mathbf{F}_{ik} - \mathbf{F}_{il} - \mathbf{F}_{im} = \mathbf{h}_0$$

where in the last equation we used force balance, $\mathbf{F}_{ij} + \mathbf{F}_{ik} + \mathbf{F}_{il} + \mathbf{F}_{im} = 0$. Thus the condition of force balance, from the requirement of mechanical stability, allows us to define a single valued function $\mathbf{h}$ on the voids. We can similarly construct $\mathbf{h}$ at all void sites.

Then

$$\hat{\sigma}_i = \sum_{j}{}' \mathbf{d}_{ij}\mathbf{F}_{ij} = \sum_{j}{}' \mathbf{d}_{ij}(\mathbf{h}_{i\nu} - \mathbf{h}_{i\mu}) = \sum_{j}{}' (\mathbf{d}_{ik} - \mathbf{d}_{ij})\mathbf{h}_{i\mu} = \sum_{\mu}{}' \mathbf{g}_{i\mu}\mathbf{h}_{i\mu}$$

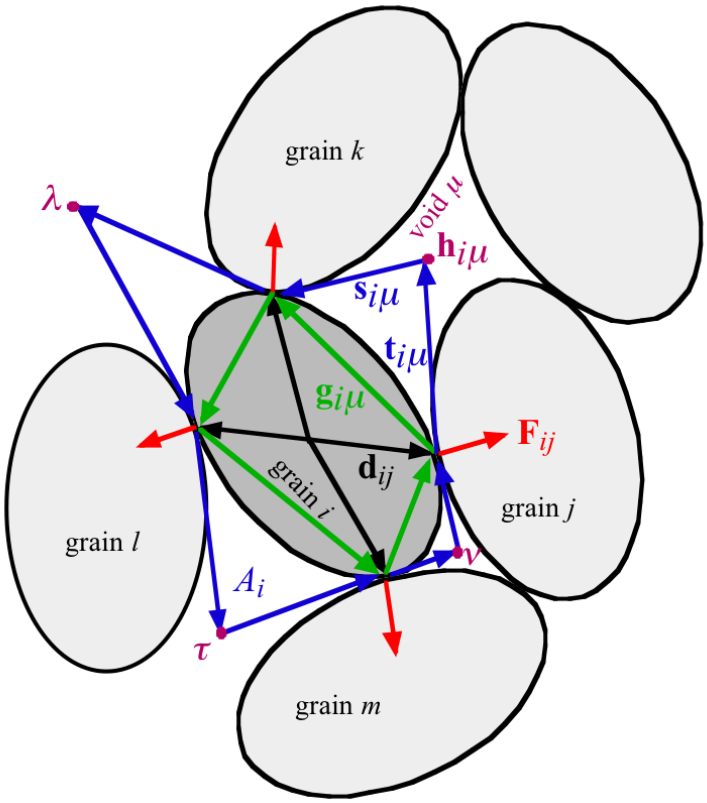


Figure 1: adapted from Henkes PhD thesis

$$\hat{\sigma}_i = \sum_{\mu}{}' (\mathbf{t}_{i\mu} + \mathbf{s}_{i\mu})\mathbf{h}_{i\mu}$$

where $\mathbf{g}$, $\mathbf{t}$ and $\mathbf{s}$ are as defined in the figure above.

The last expression represents $\hat{\sigma}_i$ in terms of a counterclockwise sum around the boundary of the area A_i associated with grain i (bounded by the blue arrows in the above figure) of the height variables $\mathbf{h}$.

If one now computes for area A

$$\hat{\mathbf{\Sigma}}_A = \sum_i \hat{\sigma}_i = \sum_{i \in A} \sum_{\mu}{}' (\mathbf{t}_{i\mu} + \mathbf{s}_{i\mu})\mathbf{h}_{i\mu}$$

one sees that the contributions from the interior boundaries in area A cancel pairwise (i.e. adding the terms from going counterclockwise around the boundary of grain i, and the terms from going counterclockwise around its neighbor grain j, there is a cancelation on the segments going through the voids common to grains i and j). Thus $\hat{\mathbf{\Sigma}}_A$ is determined just by the height variables $\mathbf{h}$ along the boundary of area A, and is insensitive to the positions of the particles in the interior of A.

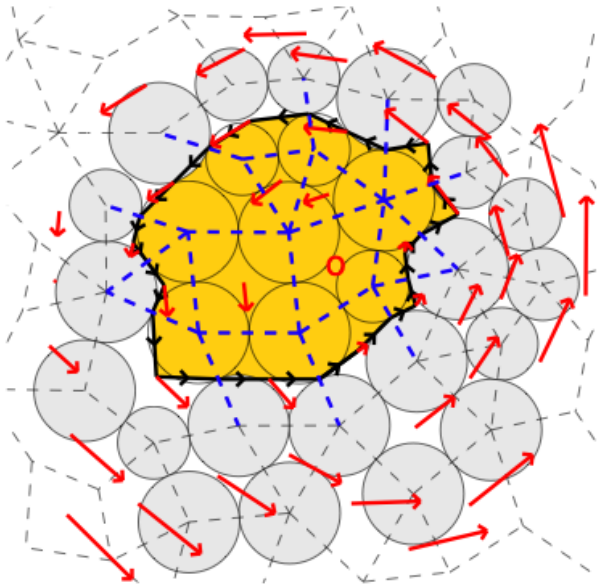


Figure 2: from Henkes PhD thesis

Similarly, if area $A = A_1 + A_2$, then one finds $\hat{\mathbf{\Sigma}}_A = \hat{\mathbf{\Sigma}}_{A_1} + \hat{\mathbf{\Sigma}}_{A_2}$.

We have thus shown that $\hat{\mathbf{\Sigma}}$ is (i) additive over subsystems, and (ii) depends on on the boundary of the system. For a system in a box with fixed boundary conditions, $\hat{\mathbf{\Sigma}}$ is therefore *conserved*. For a system in a box with periodic boundary conditions, $\hat{\mathbf{\Sigma}}$ is a topological invariant. The value of $\hat{\mathbf{\Sigma}}$ therefore cannot be changed by local rearrangements of particles (one would need some coherent global rearrangement). Although the above demonstration was done in 2D, it can be shown that the same conclusion also holds in 3D.

$\hat{\mathbf{\Sigma}}$ thus has the two properties need to try and create a statistical ensemble. This is called the stress ensemble.

Consider a box of volume V with N particles in it. Let $\{\nu\}$ be the set of mechanically stable states with a given fixed value of $\hat{\mathbf{\Sigma}}$.

As with the Edwards ensemble, we will assume a maximum entropy principle that all states ν with the same value of $\hat{\mathbf{\Sigma}}$ are equally likely.

[One can get by with a somewhat weaker condition. Suppose the system is a composite system composed of two subsystems, $S = S_1 + S_2$. Let $\nu = \nu_1 + \nu_2$ be the state consisting of ν_1 in subsystem S_1, and ν_2 in subsystem S_2. Let β_{ν_1} and β_{ν_2} be the probability weights that S_1 and S_2 are found in states ν_1 and ν_2 respectively. Then if β_ν is the probability weight that

S is found in state ν, we need to have the factorization property $\beta_\nu = \beta_{\nu_1}\beta_{\nu_2}$. See Henkes and Chakraborty, PRE]

If $\Omega(\hat{\mathbf{\Sigma}})$ is the number of states with force tensor $\hat{\mathbf{\Sigma}}$, then define

$$\hat{\alpha}_{\alpha\beta} \equiv \frac{\partial \ln \Omega}{\partial \hat{\mathbf{\Sigma}}_{\alpha\beta}}$$

$\hat{\alpha}^{-1}$ is now an effective temperature dual to $\hat{\mathbf{\Sigma}}$ and it was called by Edwards the *angoricity* tensor.

If we have the simpler case of isotropic compression with no shear, then the force tensor is diagonal, $\hat{\mathbf{\Sigma}}_{\alpha\beta} = pV\delta_{\alpha\beta}$. Denote $\Gamma = pV$. We can then define the scalar angoricity α^{-1} by

$$\alpha = \frac{\partial \ln \Omega}{\partial \Gamma}$$

Consider now a subsystem of the box that contains m particles. Viewing the remainder of the box as a reservoir, we can make the same transition to the canonical ensemble as done before. If the state ν of the m particles has a value Γ_ν, then the probability this state will occur will be

$$P_\nu \sim \exp\{-\alpha\Gamma_\nu\}$$

and the probability to find the m particles in some state with a value Γ is

$$P(\Gamma) \sim \Omega(\Gamma, m)\exp\{-\alpha\Gamma\}$$

where $\Omega(\Gamma, m)$ is the number of states of the m particles which have the the value Γ.

Numerical support for this conclusion, with a value of α that is uniform throughout the different subsystems (m particle clusters) of the box was given in Henkes, O'Hern and Chakraborty, PRL.

The partition function for the canonical ensemble of N particles is therefore a function of the angoricity

$$Q(\alpha) = \sum_\nu \mathrm{e}^{-\alpha\Gamma_\nu}$$

The state ν is defined by the geometric positions of the particles, as given by the separations of the contacting particles $\{\mathbf{r}_{ij}\}$, and the contact forces $\{\mathbf{F}_{ij}\}$. We can write the partition function as

$$Q(\alpha) = \sum_{\{\mathbf{r}_{ij}\}}\sum_{\{\mathbf{F}_{ij}\}} \exp\{-\frac{\alpha}{2}\sum_{ij} r_{ij}F_{ij}\}\delta(\text{force balance})\delta(\text{force laws})$$

where we made use of $\Gamma = pV = \frac{1}{2}\sum_{ij} r_{ij}F_{ij}$. Here $\delta(\text{force balance})$ ensures that the $\mathbf{F}_{ij}$ are related to the $\mathbf{r}_{ij}$ via the conditions of force balance, and $\delta(\text{force laws})$ ensures that the $\mathbf{F}_{ij}$ are related to the $\mathbf{r}_{ij}$ via the force law $F_{ij} = -dV_{ij}(r_{ij})/dr_{ij}$.

Now at the *isostatic point* (and *only* there) one has the special situation where the force balance equations uniquely determine the $\mathbf{F}_{ij}$, i.e. there is a one-to-one relation between the sets $\{\mathbf{r}_{ij}\}$ and the sets $\{\mathbf{F}_{ij}\}$. One can therefore use force balance to eliminate the variables $\{\mathbf{r}_{ij}\}$ and write the partition function just in terms of the $\{\mathbf{F}_{ij}\}$.

$$Q(\alpha) = \sum_{\{\mathbf{F}_{ij}\}} \exp\{-\frac{\alpha}{2} \sum_{ij} r_{ij}(\{\mathbf{F}_{ij}\}) F_{ij}\}$$

where the $\mathbf{r}_{ij}$ implicitly depend on the $\mathbf{F}_{ij}$ via the force balance constraints.

However, at the isostatic point, the particles are only just touching each other - not yet any sizeable compression into each other. Therefore all $r_{ij} \to 2R$, the diameter of a particle (we assume a monodisperse sample for simplicity). We thus get

$$Q(\alpha) = \sum_{\{\mathbf{F}_{ij}\}} \exp\{-\alpha R \sum_{ij} F_{ij}\} = \prod_{ij} \int_0^\infty dF \mathrm{e}^{-\alpha R F}$$

where the product is over all pairs of contacting particles i, j. The forces $\mathbf{F}_{ij}$ thus decouple from one another and one can sum over each F_{ij} independently. For $N z_{iso}/2$ contacts we thus get

$$Q(\alpha) = \left(\frac{1}{\alpha R}\right)^{N z_{iso}/2}$$

We can now get the equation of state. From $Q(\alpha) = \sum_\nu \exp\{-\alpha \Gamma_\nu\}$ we have,

$$\langle \Gamma \rangle = \frac{-\partial \ln Q}{\partial \alpha} = \frac{N z_{iso}}{2\alpha} \qquad \text{or} \qquad \alpha = \frac{N z_{iso}}{2\langle \Gamma \rangle}$$

This same equation of state has been found numerically in Henkes, O'Hern and Chakraborty, PRL.

Using the definite $\alpha = \partial \ln \Omega / \partial \Gamma$ we also get

$$\alpha = \partial \ln \Omega / \partial \Gamma = N z_{iso}/2\Gamma \quad \Rightarrow \quad \Omega(\Gamma, N) \sim \Gamma^{N z_{iso}/2}$$

and so the probability to find the system in a state with Γ is

$$P(\Gamma) \sim \Omega(\Gamma, N) \exp\{-\alpha \Gamma\} = \Gamma^{N z_{iso}/2} \exp\{-\alpha \Gamma\}$$

This also has been found numerically.

Finally, we have for the probability distribution of single contact forces,

$$P(F) \sim \exp\{-\alpha R F\}$$

giving an exponential distribution. In experiments and simulations, one finds that $P(F)$ appears to be exponential over some range of F, however it is not clear it if may be decaying faster than exponential at the large F tail.

Above calculation only works at the isostatic point. Other recent calculations in the "force ensemble" (Tighe, van Eerd and Vlugt, PRL 100, 238001 (2008)) have treated the hyperstatic case above jamming and find that there that the force distribution is Gaussian.

WARNING: The above results rested heavily on the assumption of equally likely states, and the factorization of density of states between a subsystem and the rest of the system. However at isostatic jamming, if jamming is indeed like a critical point, there may be a diverging correlation length ξ. If so, it is not clear how well these assumptions will apply as subsystems may always be correlated to the rest of the system via the diverging ξ.