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The distribution of forces in a granular system under external stress is a spinglass problem

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Abstract

There is now ample experimental and computational evidence that a well-defined and reproducible state can be achieved in a granular system under a repeated disturbance, e.g., if subjected to disturbance of amplitude A and frequency ω, a volume $V(A, \omega)$ is found which will be returned to if the system is subjected to A', ω' and then to A, ω. A microcanonical ensemble defines the entropy from volume V, where V equals the volume function W, just as E equals H in conventional statistical physics. A canonical version exists via a compactivity $\partial V/\partial S$. Granular systems also have a distribution of intergranular forces generated by external forces or gravity. This paper shows that the idea that the configurations are determined by the Gibbsian formula $\exp(-W(\partial S/\partial V))$ can be extended to the distribution of forces with a microcanonical condition $P(\text{external}) = \sum(\text{force moments in grains})/V$ via $\exp(-\Pi(\partial S/\partial P))$. The canonical ensemble immediately gives the exponential distribution of intergranular forces, found experimentally. The distribution must depend on the configuration and any physical property will have a value averaged over configurations, i.e. will give rise to a spinglass problem.

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Introduction

Powders are the simplest case of a jammed state, and under the correct conditions are subject to a version of statistical mechanics. The simplest powders, and the most common, have grains possessing high friction and low compressibility, e.g., sand. If such a powder is subjected to a shaking disturbance of amplitude A and frequency ω, it will take up a volume V:

$$V = V(A, \omega). \tag{1}$$

Suppose W is the function of all the surfaces and orientation of the grains which determines the volume V, then the central hypothesis [1] is that distribution function is

$$e^{-S}\delta(V - W)\Theta \tag{2}$$

where e^{-S} is the normalization and Θ is the condition that all grains are locked in touching neighbours (i.e., jammed). Equation (2) seems to survive experiment and simulation well [2]. The microcanonical (1.2) becomes the canonical

$$\exp[(Y - W)/X]\Theta \tag{3}$$

where

$$X = \partial V/\partial S \tag{4}$$

$$S = \log \int \delta(V - W)\, \Theta \,\mathrm{d}\, \text{all}. \tag{5}$$

A powder is normally kept in a jammed condition by external forces, for example being in a box, kept down by gravity. The simplest form is to imagine the box exerting external pressure on the system or having the powder within a membrane and subjecting it to hydrostatic pressure. This is simpler than the inhomogeneity of gravity and so we adopt it.

Now our process of shaking or sending some kind of disturbance through the powder, our A, ω above, will not only establish a regime of configuration, but also a force distribution between the grains. Although one could subject the system to an external stress field on its boundaries, for simplicity we take just a hydrostatic pressure to generate the forces. There is now the subtlety that the configuration can be first fixed (sand goes to sandstone) and then the force system set up, a spin glass problem, or, simpler, consider the perfectly physical case in which the disturbance sets up both configurations and force patterns. Under these circumstances, the entropy will depend on V and P, where P is the external pressure and this relates to the stress (force moments) of the grains, i.e., there will be a function Π such that $P = \Pi$ and $V = W$. The fomula for Π is

$$\Pi = \sum_{\alpha,\beta} f^{\alpha\beta} r^{\alpha\beta} / V^{\alpha} \tag{6}$$

where $f^{\alpha\beta}$ is the force acting on grain β from grain α, V^{α} is the grain volume and $r^{\alpha\beta}$ is the vector from the centroid of contacts to the point of contact of α and β. We only consider the pressure for simplicity, but we could use the whole stress tensor and have

$$P_{ij} = \Pi_{ij} = \sigma_{ij}. \tag{7}$$

We emphasize that P is external; it has nothing to do with the kinematic pressure which is zero in a powder. The entropy S is now

$$S = S(V, P, N) \tag{8}$$

where we write N on the assumption that all grains are similar, but essentially w.l.o.g. Moving from the microcanonical to the canonical ensemble, we have the probability distribution

$$e^{-S}\delta(V - W)\delta(P - \Pi)\Theta_V \Theta_P \tag{9}$$

becoming

$$\exp[(-S + (V - W))\partial S/\partial V + (P - \Pi)\partial S/\partial P]\Theta_V \Theta_P. \tag{10}$$

This is the analogue in ordinary statistical mechanics of

$$\exp[(S - (E - H))\partial S/\partial E] \tag{11}$$

$$-\frac{F}{T} = S - E\frac{\partial S}{\partial E} = S - \frac{E}{T} \tag{12}$$

or

$$F = E - TS \tag{13}$$

is

$$S - V\frac{\partial S}{\partial V} - P\frac{\partial S}{\partial P}. \tag{14}$$

Earlier work has defined the 'compactivity'

$$\frac{1}{X} = \frac{\partial S}{\partial V} \tag{15}$$

and we name Z the angoricity [3]:

$$\frac{1}{Z} = \frac{\partial S}{\partial P}. \tag{16}$$

The canonical distribution is therefore

$$\wp = \exp[-S + V/X + P/Z - W/X - \Pi/Z]\Theta_V\Theta_P. \tag{17}$$

The Θ functions ensure that the grains are in a jammed configuration via Θ_V, and Θ_P contains the restriction on the $f^{\alpha\beta}$ via Newton's laws, i.e.,

$$\Theta_P = \prod_{\alpha\beta}\delta\big(f_i^{\alpha\beta} + f_i^{\beta\alpha}\big)\delta\left(\sum_\beta \varepsilon_{ikl} f_k^{\alpha\beta} r_l^{\alpha\beta}\right)\prod_\alpha \delta\left(\sum_\beta f_i^{\alpha\beta}\right). \tag{18}$$

In the latter two δs, we have omitted the body force which in the full version would be there from any external body couple and from gravity.

Thus, without the detailed calculations in the literature [4], we have obtained an exponential distribution of forces, for Π it is linear in the $f_i^{\alpha\beta}$, which, since they are approximately parallel to the $r_i^{\alpha\beta}$, gives

$$|f^{\alpha\beta}||r^{\alpha\beta}| \qquad \text{for } \; f^{\alpha\beta}\cdot r^{\alpha\beta}. \tag{19}$$

Distribution (10) corresponds to the simultaneous shaking of the powder and applying a variable external force pattern whose mean is P. Under the condition described in the introduction this is not realistic. Once the shaking is over, the external pressure will not alter the configuration so the pressure function Π will be a function of the volume function. Thus, if we study any physical quantity S say, we must first calculate S and then average over W. This is a spin glass situation and is much more difficult than using distribution (10). For example if we need the mean entropy of the force

$$\langle S_F\rangle = \int S_F(W)\,\mathrm{e}^{-\frac{W}{X}}\,\mathrm{d}W \Big/ \int \mathrm{e}^{-\frac{W}{X}}\,\mathrm{d}W \tag{20}$$

$$= \int Z\left[\log\int e_{dp}^{-\Pi/Z}\right]\mathrm{e}^{-W/X} \Big/ \int \mathrm{e}^{-W/X}\,\mathrm{d}W. \tag{21}$$

The log makes the integral very difficult, and I have not yet found a simple approach. If however one integrates (10), assuming simultaneous averaging, it becomes easy to offer a model.

The distribution

Experiment gives clear confirmation of the exponential distribution [4], and can be fitted to curves like $f^\alpha \exp(-f/m)$ (although the behaviour near $f \cong 0$ is not clear yet) where m is a constant.

Any particular $f_i^{\alpha\beta}$ is related to $f_i^{\beta\alpha}$, but also to the other $f_i^{\alpha y}$ via $\sum_\beta f_i^{\alpha\beta} = 0$. Thus, there is still a calculation required to obtain the probability distribution of a single force. Here we will make a crude model and write

$$P = \sum_\alpha \gamma f^\alpha. \tag{22}$$

A straightforward calculation is

$$W = \sum w^\alpha \tag{23}$$

$$S = 3N \log P + N \log V + \text{constants} \tag{24}$$

here, 3 and unity coming simply from assuming the integration is over $\mathrm{d}W^\alpha$ and $f^2 \mathrm{d}f$. Thus this very crude estimate gives

$$S = N \log(P^\alpha V^b) + \text{constants} \tag{25}$$

and

$$\frac{\partial S}{\partial V} = \frac{1}{X} = \frac{bN}{V} \tag{26}$$

$$\frac{\partial S}{\partial P} = \frac{1}{Z} = \frac{aN}{P}. \tag{27}$$

Of course, in reality, the calculation is much more complex, but granular systems are ensembles of crude objects and it does not seem worth making really detailed calculations at this stage. A spin glass treatment at the crudest level needs a form for σ(W). The simplest form, chosen essentially to be illustrative, is

$$\sigma = \sigma_\sigma + \beta W. \tag{28}$$

This leads to

$$\bar{s} = \int_\alpha^\infty \mathrm{d}W \, \mathrm{e}^{-W/x} \log \int \mathrm{d}\sigma \frac{\mathrm{e}^{-(p-\sigma)/x - \beta W}}{\int_\alpha^\infty \mathrm{d}W \, \mathrm{e}^{-W/x}} \tag{29}$$

where, since this is an illustrative calculation, Jacobians have been put unit.

After calculation one reaches the distribution of forces

$$\frac{\mathrm{e}^{-\sigma}}{\int_\alpha^\infty \mathrm{d}W \, \mathrm{e}^{-W/x}} \tag{30}$$

and equation (27) is replaced by

$$Z = P + \beta V. \tag{31}$$

Conclusion

One can see three regimes of granular systems: (1) suspensions, really part of hydrodynamics. (2) Granular systems where the history of formation is still apparent, e.g. a sand pile. In these, ad hoc theories must be constructed. (3) True statistically defined systems where the rules of statistical mechanics can be modified to allow for the dominance of a jammed state achieved by motions dominated by friction. Such systems have no third law, there is a whole new statistical mechanics emerging from the point which in conventional, thermal, statistical mechanics is $T = 0$, $S = 0$.

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