Granular paper club
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Michael Engel
Numerical Calculation of Granular Entropy

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We present numerical simulations that allow us to compute the number of ways in which \( N \) particles can pack into a given volume \( V \). Our technique modifies the method of Xu, Frenkel, and Liu [Phys. Rev. Lett. 106, 245502 (2011)] and outperforms existing direct enumeration methods by more than 200 orders of magnitude. We use our approach to study the system size dependence of the number of distinct packings of a system of up to 128 polydisperse soft disks. We show that, even though granular particles are distinguishable, we have to include a factor \( 1/N! \) to ensure that the entropy does not change when exchanging particles between systems in the same macroscopic state. Our simulations provide strong evidence that the packing entropy, when properly defined, is extensive. As different packings are created with unequal probabilities, it is natural to express the packing entropy as \( S = -\sum p_i \ln p_i - \ln N! \), where \( p_i \) denotes the probability to generate the \( i \)th packing. We can compute this quantity reliably and it is also extensive. The granular entropy thus (re)defined, while distinct from the one proposed by Edwards [J. Phys. Condens. Matter 2, SA63 (1990)], does have all the properties Edwards assumed.

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Questions/Motivations

• Granular entropy is defined as the logarithm of the number of distinct mechanically stable packings.

• Can this be measured? (it is a “miracle” that is can)

• Along the lines we will learn about sampling high-dimensional energy landscapes. This can be useful in many circumstances.

• Frenkel: “[this work] is not just an interesting intellectual exercise”
Direct Determination of the Size of Basins of Attraction of Jammed Solids

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We propose a free-energy-based Monte Carlo method to measure the volume of potential-energy basins in configuration space. Using this approach we can estimate the number of distinct potential-energy minima, even when this number is much too large to be sampled directly. We validate our approach by comparing our results with the direct enumeration of distinct jammed states in small packings of frictionless spheres. We find that the entropy of distinct packings is extensive and that the entropy of distinct hard-sphere packings must have a maximum as a function of packing fraction.

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Model system

- 2D system of quasi-hard particles.
- System is polydisperse with Gaussian distribution.
- Interaction potential:

\[
\varphi(r_{ij}) = \begin{cases} 
+\infty, & r_{ij} < d_{ij}^\text{HD} \\
\text{WCA}(r_{ij} - d_{ij}^\text{HD}), & d_{ij}^\text{HD} < r_{ij} < d_{ij}^S \\
0, & r_{ij} > d_{ij}^S 
\end{cases}
\]

- Idea: Combine concepts from hard particles and avoid problems with discontinuities
Energy landscape basins of attraction

- $2N$-dimensional configuration space
- Each point is assigned a local minimum.
- Average hyper-volume of the basin of attraction:

\[ \langle v \rangle (N, \phi) \equiv \frac{1}{\Omega(N, \phi)} \sum_{i=1}^{\Omega(N, \phi)} v_i = \frac{V_{\text{acc}}(N, \phi)}{\Omega(N, \phi)} \]

Configurational integral of hard-core fluid (known, see: [30])

Number of minima
Sample basin voluming ("tricky part")

- Generate random configuration
- Quench in local minima
- Perform Einstein integration using thermodynamic integration:

\[ F_i(N, \phi) = F_{\text{Harmonic}}(N, \phi) - \frac{1}{2} \int_0^{k_i^{\text{max}}} dk \langle u^2(k) \rangle, \]

where we introduce the free energy \( F_i(N, \phi) \equiv -\ln v_i(N, \phi) \) and where \( \langle u^2(k) \rangle \) denotes the canonical average of the square of the displacement vector \( u \) from the lattice positions corresponding to the minimum \( i \). The energy cost for such a displacement is \( ku^2/2 \) if \( u \) is inside the basin \( i \), and infinite otherwise. For \( k = k_i^{\text{max}} \), \( \langle u^2(k) \rangle \) is estimated by static Monte Carlo sampling. For all other values of \( k \) we use a Markov-chain Monte Carlo sampling, combined with parallel tempering (see, e.g., [22]) to speed up the convergence. We choose \( k_i^{\text{max}} \) such that 85%-95% of random displacements generated from minimum \( i \) are within its basin of attraction.
Method

• Select packing density of hard-core system with up to 128 particles

• Generate 1000 equilibrium hard-disk patterns (can only be done in the fluid)

• Turn on attraction and sample: density jumps, system jams

• Quench to local minimum using FIRE algorithm (Bitzek et al. PRL 2006)
Discussion

• Not all minima are found with equal probability.

• In fact, minima are found with probability equal to their volume (Boltzmann entropy):

\[
S = \ln \Omega \quad \Rightarrow \quad S^* = -\sum_i p_i \ln p_i.
\]

• Poor (impossible) sampling of small basins
Fitting basin volume distribution

We then fit the observed distributions $B$ with a three-parameter generalized normal distribution $p(F|\bar{F}, \alpha, \beta)$ that reads

$$p(F|\bar{F}, \alpha, \beta) \equiv \frac{\beta}{2\alpha \Gamma(1/\beta)} e^{-((|F-\bar{F}|/\alpha)^\beta}, \quad (6)$$

where $\Gamma(x)$ is the Euler gamma function (see Fig. 1). In Eq. (6), the mean of $F$ is $\bar{F}$ and its variance is $\alpha^2 \Gamma(3/\beta)/\Gamma(1/\beta)$. In the limit $\beta \to 2$, we recover the normal distribution with width $\alpha$.

- alpha scales linearly
- beta tends to 2 for large $N$
- use fit to obtain average basin volume
Main result

- Size ratio of soft (S) and hard (HD) disks does not matter (robust!)

- Have to consider disks indistinguishability. NOT a quantum effect.

- Huge number of minima: $O(10^{250})$
What is granular entropy?

In what follows, we shall make a distinction between \( \ln \Omega \) and the granular entropy. The reason is twofold: first of all, as different packings have different basins of attraction, they are \textit{not} populated equally. Yet, only when all packings are equally likely can we expect \( \ln \Omega \) to be a measure for the granular entropy. Hence, we should use the more general expression for the entropy of systems with states that are not equally likely,

\[
S^* = -\sum_i p_i \ln p_i = -\langle \ln v \rangle_B + \ln V_{\text{acc}}(N, \phi_{\text{HD}}).
\]

Boltzmann weighted average Basin hypervolume

Hard disk phase space volume

\( N.B.: \) granular entropy is extensive!

Edwards's hypothesis of the existence of a meaningful granular entropy therefore survives when the condition that all granular packings are equally likely is dropped [35].
Turninng intractable counting into sampling: computing the configurational entropy of three-dimensional jammed packings

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We report a numerical calculation of the total number of disordered jammed configurations $\Omega$ of $N$ repulsive, three-dimensional spheres in a fixed volume $V$. To make these calculations tractable, we increase the computational efficiency of the approach of Xu et al. (Phys. Rev. Lett. 106, 245502 (2011)) and Asenjo et al. (Phys. Rev. Lett. 112, 098002 (2014)) and we extend the method to allow computation of the configurational entropy as a function of pressure. The approach that we use computes the configurational entropy by sampling the absolute volume of basins of attraction of the stable packings in the potential energy landscape. We find a surprisingly strong correlation between the pressure of a configuration and the volume of its basin of attraction in the potential energy landscape. This relation is well described by a power law. Our methodology to compute the number of minima in the potential energy landscape should be applicable to a wide range of other enumeration problems in statistical physics, string theory, cosmology and machine learning, that aim to find the distribution of the extrema of a scalar cost function that depends on many degrees of freedom.
Same story in 3D (spread out over 18 pages)

- Optimization and speed-ups (e.g. parallel tempering for thermodynamic integration)

**FIG. 1:** Entropy as a function of system size $N$ for two (Ref. [34]) and three-dimensional (this work) jammed sphere packings. Dashed curves are lines of best fit of the form $S = aN$. 
What is Matthias’ take on this?
Follow-up #2

Structural analysis of high-dimensional basins of attraction

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We propose an efficient Monte Carlo method for the computation of the volumes of high-dimensional bodies with arbitrary shape. We start with a region of known volume within the interior of the manifold and then use the multi-state Bennett acceptance-ratio method to compute the dimensionless free-energy difference between a series of equilibrium simulations performed within this object. The method produces results that are in excellent agreement with thermodynamic integration, as well as a direct estimate of the associated statistical uncertainties. The histogram method also allows us to directly obtain an estimate of the interior radial probability density profile, thus yielding useful insight into the structural properties of such a high dimensional body. We illustrate the method by analysing the effect of structural disorder on the basins of attraction of mechanically stable packings of soft repulsive spheres.
Another take and why we should really care (energy landscape in molecules, cosmology, string theory, …)

- Collaboration with David J. Wales

- “In this Letter we show that **MBAR** *(multi-state Bennet acceptance ratio)* can be used, **not only** to arrive at an **accurate estimate of a high-dimensional, non-convex volume**, but that it **also** can be used to probe the **spatial distribution of this volume**.”

- “We thus observe that the structural **isotropy and high degree of rotational symmetry** in the crystal […] is reflected in the **isotropy and spherical symmetry** of the basin around the minimum.”