## Edwards ensemble and glasses

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Granular matter
Random close packing (RCP)
Bernal packings (1960)

Glasses

## Applications



1. Edwards ensemble for grains and glass theory


Theoretical approach I: Statistical mechanics (Edwards' ensemble)

## Constraint optimization problem

$$
\mathcal{Z}(X, T)=\int \exp [-\mathcal{W}(\vec{x}) / X] \exp [-\mathcal{H}(\vec{x}, \vec{f}) / T] \mathcal{D} \vec{x} \mathcal{D} \vec{f}
$$

Minimize volume ( $\mathrm{X}=0$ ) with constraint of force balance ( $\mathrm{T}=0$ ) and non-overlaping.

| OPTIMIZATION | STATISTICAL PHYS | EDWARDS |
| :---: | :---: | :---: |
| instance | sample | packing |
| cost function | energy | volume |
| optimal configuration | ground state | RCP at X=0 |
| minimal cost | ground state energy | minimal volume |

Theoretical approach II: Mean field theory of jammed hard-sphere (remnant of RSB solution from replica theory)


- Approach jamming from the liquid phase.
- Predict a range of RCP densities $\left[\phi_{\mathrm{th}}, \phi_{\mathrm{GCP}}\right] \approx[0.64,0.68]$
- Mean field theory based on RSB solution in the glass phase.
(un)Commonalities between Edwards ensemble and RT: 3d



## Very difficult in practice: very small range for 3d equal-size spheres



## 1. Full solution: Constraint optimization problem

$$
\mathcal{Z}(X, T)=\int \exp [-\mathcal{W}(\vec{x}) / X] \exp [-\mathcal{H}(\vec{x}, \vec{f}) / T] \mathcal{D} \vec{x} \mathcal{D} \vec{f}
$$

## $\mathrm{T}=0$ and $\mathrm{X}=0$ optimization problem

## $\downarrow$

2. Approximation: Decouple forces from geometry.

$$
\mathcal{Z}(X, T)=\int \exp [-\mathcal{W}(\vec{x}) / X] \mathcal{D} \vec{x} \times \int \exp [-\mathcal{H}(\vec{f}) / T] \mathcal{D} \vec{f}
$$

3. Edwards for volume ensemble + Isostaticity

$$
\mathcal{Z}(X, Z)=\int_{Z}^{6} \exp \left[-\frac{w(z)}{X}\right] g(z) d z
$$

Song, Wang, Jin, Makse, Physica A (2010)
4. Cavity method for force ensemble

$$
\mathcal{H}=\sum_{a=1}^{N}\left[\left(\sum_{b,(a b) \in E} f_{a b} \hat{n}_{a b}\right)^{2}\right]
$$

Bo, Mari, Song, Makse (2013)

## The Volume function is the Voronoi volume



## "Easily" generalizable to other systems


equal size
spheres

ellipsoids, spherocylinders, non-convex particles, rods, sphere/ellipsoids mixtures, etc.
any dimension

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## Analytical formula for Voronoi boundary



$$
W_{i}=\frac{1}{3} \oint\left(\frac{1}{2 R} \min _{j} \frac{r_{i j}}{\cos \theta_{i j}}\right)^{3} d s
$$

Important: global minimization. Reduce to one-dimension

## Analytical formula for Voronoi boundary



Important: global minimization. Reduce to one-dimension

## Analytical formula for Voronoi boundary



Important: global minimization. Reduce to one-dimension

## Analytical formula for Voronoi boundary



Important: global minimization. Reduce to one-dimension

## Average free-volume per particle

$$
w=\int_{1}^{\infty}\left(c^{3}-1\right) p(c) d c=\int_{0}^{1}\left(c^{3}-1\right) d P_{>}(c)
$$



Geometrical interpretation of cumulative dist:

$$
\begin{gathered}
P_{>}(c) \\
-\frac{\partial P_{>}(c)}{\partial c}=p(c)
\end{gathered}
$$

Probability to find all particles outside excluded volume and surface:

$$
V^{*}(c) \quad S^{*}(c)
$$

## Mean-field approximation analogous to decorrelation principle

particles belong to bulk or in contact:

$$
P_{>}(c)=P_{B}(c) \times P_{c}(c)
$$

$$
g_{2}(r) \simeq \frac{z}{\rho S_{d-1}} \delta(r-1)+\Theta(r-1)
$$



Similar to car parking
$V^{*}(c)$ problem (Reni, 1960).
Probability to find a spot with $V^{*}(c)$ in a volume V

Particle gas

$$
P\left(V^{*}\right)=\left(1-V^{*} / V\right)^{N} \rightarrow e^{-\rho V^{*}}
$$

## Calculation of $\mathrm{P}_{>}(\mathrm{c})$

Particles are in contact and in the bulk:

$$
P_{>}(c)=P_{B}(c) \times P_{c}(c)
$$



Bulk term:

$$
P_{B}(c)=e^{-\rho V^{*}(c)} \quad \rho(w)=\frac{1}{w}
$$

mean free volume density
Contact term:

$$
P_{C}(c)=e^{-\rho_{s} S^{*}(c)} \rho_{s}(z)=\frac{1}{\left\langle S^{*}\right\rangle}=\frac{\sqrt{3}}{4 \pi} z
$$

$z=$ geometrical coordination number

## Average Voronoi volume

$$
P_{>}(c)=P_{B}(c) \times P_{c}(c)
$$

$$
P_{>}(c)=\exp \left[-\frac{1}{w}\left(\left(c^{3}-1\right)-3\left(1-\frac{1}{c}\right)\right)-\frac{\sqrt{3}}{2} z\left(1-\frac{1}{c}\right)\right]
$$

Self-consistent equation:

$$
w=\int_{0}^{1}\left(c^{3}-1\right) d \exp \left[-\frac{1}{w}\left(\left(c^{3}-1\right)-3\left(1-\frac{1}{c}\right)\right)-\frac{\sqrt{3}}{2} z\left(1-\frac{1}{c}\right)\right]
$$

equal to zero
$w=\frac{2 \sqrt{3}}{z} \xrightarrow{ } \begin{aligned} & \text { represent the av } \\ & \text { a single particle }\end{aligned}$

## Prediction: volume fraction vs z

free volume

volume function

$$
\phi=\frac{z}{z+2 \sqrt{3}}
$$

Equation of state agrees well with simulations

| RCP |
| :---: |
| $z=6$ |
| $w=\frac{1}{\sqrt{3}}$ |
| $\phi=\frac{6}{6+2 \sqrt{3}}$ |
| $\phi=.634$ | and experiments



Definition of jammed state: geometric coordination z bounded by mechanical coordination Z

$$
\underset{\mu=\infty}{4=d}+1 \leq \underset{\mu=0}{Z} \leq \underset{\mu=6}{2 d=6}
$$

$$
z \leq 2 d
$$

$N d$ positions $z N / 2{ }_{\text {constraints }}^{\text {geometrical }}$

$$
\left|r_{i}-r_{j}\right|=2 R
$$

## Edwards phase diagram for hard spheres



## Jammed packings in high dimensions

Rigorous bounds
Minkowsky lower bound: $\phi \sim 2^{-d}$
Kabatiansky-Levenshtein upper bound: $\phi \sim 2^{-0.5990 \ldots d}$

Question: what's the density of RCP in high dimensions? Conjecture: are disordered packings more optimal than ordered ones?

## Conjecture: $P_{>}(c)$ becomes valid in the high-dimensional limit

(I) Theoretical conjecture of $g_{2}$ in high $d$ (neglect correlations)

Torquato and Stillinger, Exp. Math., 2006

$$
g_{2}(r) \simeq \frac{z}{\rho S_{d-1}} \delta(r-1)+\Theta(r-1)
$$


(II) Factorization of $P_{>}(c)$

$$
P_{>}(c)=P_{B}(c) P_{C}(c)
$$

## Comparison with other theories

Edwards' theory

$$
\phi \sim \frac{4 d}{3} 2^{-d}
$$

Isostatic packings $(z=2 d)$ with unique volume fraction

Jin, Charbonneau, Meyer, Song, Zamponi, PRE (2010)

Agree with Minkowski lower bound

Glass transition RT

$$
\phi \in\left[6.26 d 2^{-d}, d \ln (d) 2^{-d}\right]
$$

Parisi and Zamponi, Rev. Mod. Phys. (2010)

Isostatic packings ( $z=2 d$ ) ranging volume fraction increases with dimensions

No unified conclusion at the mean-field level (infinite $d$ ). Neither dynamics nor jamming. Does RCP in large $d$ have higher-order correlations missed by theory?: Test of replica th. Edwards solution seems to corresponds to $\phi_{t h}$. Higher entropy state.

## Generalizing the theory of monodisperse sphere packings



Distribution of radius $P(r)$ Distribution of angles $P(\hat{s})$

## Extra degree of freedom

treated as in Onsager 1949

## Optimizing random packings in the space of object shapes

- Simulation results on packings of ellipsoids:
$>$ Ellipsoids pack denser than spheres
> Peak at aspect ratio

$$
\alpha \approx 1.4
$$

$>$ Spheres appear as a singular limit


Donev et al, Science 2004

## Edwards prediction

- Non-spherical objects:

$$
\bigcap_{d} \downarrow L \quad \alpha=\frac{L}{d}
$$

$$
\phi(\alpha)=\phi(Z(\alpha), \alpha)
$$

$$
z<2 d_{f}
$$

## Edwards prediction

- Non-spherical objects:

$$
\bigcap_{d}\left\lfloor L \quad \alpha=\frac{L}{d}\right.
$$

$$
\phi(\alpha)=\phi(Z(\alpha), \alpha)
$$

$$
\phi(Z, \alpha)
$$

Statistical theory of
Voronoi volume

$$
z<2 d_{f}
$$

## Edwards prediction

- Non-spherical objects:

$$
\bigcap_{d} \downarrow L \quad \alpha=\frac{L}{d}
$$



$$
\phi(Z, \alpha)
$$

$Z(\alpha)$

Statistical theory of Voronoi volume

Evaluating the probability of degenerate configurations: ellipsoids are hypoconstrained

$$
z<2 d_{f}
$$

## Voronoi for non-spherical shapes



## General non-spherical shapes




## Spherocylinders

- Separation lines:

- Four different interactions:
- Line - Line
- Line - Point
- Point - Line
- Point - Point

Exact equation for each case $\longrightarrow$ analytic expressions for VB

## Calculation of coordination number: Degenerate configurations

- Mechanical equilibrium:
- 3 force equations
- 2 torque equations (torque along symmetry axis vanishes)
Linearly independent?
$Z_{c}=2 d_{f}=10$

$\longrightarrow \quad$ Effective number of degrees of freedom can be reduced!


## Degenerate configurations

- Mechanical equilibrium:
- 3 force equations
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Linearly independent?

$\longrightarrow \quad$ Effective number of degrees of freedom can be reduced!


## Degenerate configurations

- Mechanical equilibrium:
- 3 force equations
- 2 torque equations (torque along symmetry axis vanishes)
Linearly independent?


Maximal degenerate configuration: Condition of force balance automatically implies torque balance!

$$
\longrightarrow \quad Z(\alpha)=2\left\langle\tilde{d}_{f}(\alpha)\right\rangle
$$

## Theoretical predictions




## Simulations

| spherocylinder | Abreu et al. 2003 | $\bigcirc$ |
| :---: | :---: | :---: |
| \&M candy | Donev et al. 2004 | $\nabla$ |
| spherocylinder | Lu et al. 2010 |  |
| spherocylinder | Jia et al. 2007 |  |
| spherocylinder | Williams et al. 2003 | $\square$ |
| me | Schreck et al. 2011 | $\Delta$ |
| dimer | Faure et al. 2009 |  |
| spherocylinder | Kyrylyuk et al. 2011 | $\nabla$ |
| spherocylinder | Bargiel et al. 2008 | $>$ |
| oblate ellipsoid | Donev et al. 2004 | 4 |
| spherocylinder | Wouterse et al. 2009 | $\bigcirc$ |
| prolate ellipsoid | Donev et al. 2004 | - |
| spherocylinder | Zhao et al. 2012 | $\bigcirc$ |

## Results for packing fraction: dimers



## Results for packing fraction: spherocylinders



## Edwards phase diagram for many shapes



## RCP is not singular: analytical continuation of${ }^{4}$ spheres

## Summary

## Ode to Edwards!

1. Edwards ensemble to predict RCP for spheres.
2. Edwards ensemble for non-spherical particles.
3. Edwards ensemble for packings in large dimensions to compare with replica theory of hard sphere glasses.
4. Edwards replica trick or cavity method for proper average over quenched disorder for force distribution for any system: spheres, non-spheres, friction and frictionless, any dimension.
5. Extending Maxwell argument: Cavity method at RS level for solution-no solution transition to calculate $Z_{c}$ from frictionless isostatic grains to frictional grains.
6. Edwards CAVEAT: 1-5 done at expense of drastic (yet controlled) approximations.

## Cavity Method for Force Transmission

$$
\mathcal{Z}(X, T)=\int \exp [-\mathcal{W}(\vec{x}) / X] \mathcal{D} \vec{x} \times \int \exp [-\mathcal{H}(\vec{f}) / T] \mathcal{D} \vec{f}
$$

Edwards volume ensemble predicts: $\phi(Z)$

Cavity method predicts Z: $\quad Z(\alpha)$
and Force Distribution: $\quad P(f)$

# Force transmission problem: back to Edwards (simplest model) 

Edwards model = q-model = annealed disorder average

Fix $Z=4$

> Find $P(f)$
with constraint

$$
\vec{f}=-\left(\overrightarrow{f_{1}}+\overrightarrow{f_{2}}+\overrightarrow{f_{3}}\right)
$$



## Boltzmann equation for $P(f)$



Boltzmann equation:
assuming uncorrelated forces (MF)
$P(f)=\int P\left(f_{1}, \lambda_{1}\right) P\left(f_{2}, \lambda_{2}\right) \sqrt{\tau\left(\lambda_{1}, \lambda_{2}\right)} \delta\left(f-\lambda_{1} f_{1}-\lambda_{2} f_{2}\right) d \lambda_{1} d \lambda_{2} d f_{1} d f_{2}$
Edwards: "Tiresomely complicated function well annealed disorder $\longrightarrow$ modelled by integrating between 0 and 1 "

Fourier transform:

$$
P(f)=\frac{f}{p} e^{-\frac{f}{p}}
$$

## Annealed versus quenched disorder

Experimentally: first find the distribution for a fixed (quenched) packing, then average over the ensemble of packings
Average must be carried over a physical observable: free energy, not the partition function.
quenched disorder

$$
F=-\underset{\downarrow}{-k T \overline{\ln Z}}
$$

$$
F=-k T \ln \bar{Z}
$$

Granular matter:
Performed average over forces then over contact network

## Building the factor graph of contacts from a packing



$$
\chi_{a}\left(\left\{f^{n}, f^{t}, \hat{n}^{a}, \hat{t}^{a}\right\}_{\partial a}\right)=\delta\left(\sum_{i \in \partial a} \vec{f}_{i}^{a}\right) \delta\left(\sum_{i \in \partial a} \vec{r}_{i}^{a} \times{\overrightarrow{f_{i}}}^{a}\right) \times \prod_{i \in \partial a} \Theta\left(f_{i}^{n}\right) \Theta\left(\mu f_{i}^{n}-f_{i}^{t}\right)
$$

Constraint: force balance + torque balance + repulsive ${ }^{40}$ Coulomb

## Compute marginal belief for a fix contact network <br> $\mathrm{Q}^{i}\left(f_{i}^{n}, f_{i}^{t}\right)$

Cavity field:
no average over $n_{j}$

$$
\begin{gather*}
\mathrm{Q}^{a \rightarrow i}\left(f_{i}^{n}, f_{i}^{t}\right)=\frac{1}{Z^{a \rightarrow i}} \int \mathrm{~d} \hat{t}_{i} \prod_{\substack{j \in \partial a-i \\
c=\partial j-a}} \mathrm{~d} f_{j}^{n} \mathrm{~d} f_{j}^{t} \mathrm{~d} \hat{t}_{j} \mathrm{Q}^{c \rightarrow j}\left(f_{j}^{n}, f_{j}^{t}\right) \chi_{a}\left(\left\{f^{n}, f^{t}, \hat{n}, \hat{t}\right\}_{\partial a}\right) \\
\mathrm{Q}^{i}\left(f_{i}^{n}, f_{i}^{t}\right)=\frac{1}{Z^{i}} \mathrm{Q}^{a \rightarrow i}\left(f_{i}^{n}, f_{i}^{t}\right) \mathrm{Q}^{b \rightarrow i}\left(f_{i}^{n}, f_{i}^{t}\right), \quad\{a, b\}=\partial i \tag{41}
\end{gather*}
$$

# Force probability over an ensemble of random graphs <br> $P\left(f^{n}\right)$ 

Degree distribution
Joint distribution of contacts positions on one particle Solved with Population Dynamics

$$
\mathcal{Q}\left(\mathrm{Q}^{\rightarrow}\right)=\frac{1}{\mathcal{Z}} \sum_{z} z \stackrel{\mathrm{R}}{ }(z) \int \underset{\sim}{\boldsymbol{Z}}\left(\left\{\hat{n}_{j}\right\}\right) \prod_{j=1}^{z-1} \mathrm{~d} \hat{n}_{j} \mathrm{DQ}^{\rightarrow j} \mathcal{Q}\left(\mathrm{Q}^{\rightarrow j}\right) \delta\left[\mathrm{Q}^{\left.\rightarrow-\mathcal{F}_{\rightarrow}\left(\left\{\mathrm{Q}^{\rightarrow j}\right\}\right)\right]}\right.
$$

$$
\mathrm{P}\left(f^{n}, f^{t}\right)=\left\langle\mathrm{Q}^{i}\left(f^{n}, f^{t}\right)\right\rangle=\frac{1}{\mathrm{Z}}\left[\int \mathrm{DQ}^{a \rightarrow i} \mathcal{Q}\left(\mathrm{Q}^{a \rightarrow i}\right) \mathrm{Q}^{a \rightarrow i}\left(f^{n}, f^{t}\right)\right]^{2}
$$

Prediction: $P(f) \sim f^{\theta} \quad \theta=0 \quad$ signature of jamming



## The Population Dynamics Algorithm

- $\mathrm{G}(\mathrm{V}, \mathrm{E})$, Initialize all cavity fields $\left\{\psi^{i \rightarrow a}\left(f_{i}\right)\right\}$.
- Draw an integer z with (edge-perspective) degree distribution $\mathrm{P}(\mathrm{z})$.
- Then pick at random z-1fields $\psi^{j \rightarrow b}\left(f_{j}\right)$ from the population of N fields.
- Generate a set of relative contact directions $n_{i(1)}, \ldots, n_{i(z-1)}$ with uniform distribution ; Particles do not overlap.
- update the new cavity field $\psi^{i \rightarrow a}\left(f_{i}\right)$ by using the incoming fields according to cavity equation.
- Update all cavity fields to generate a new population. Rescale $\langle\mathrm{f}\rangle=$ const. Run until convergence, or until the number of iterations exceeds $\mathrm{T}_{\text {max }}$.


## Force probability over an ensemble of random graphs $P_{\mu}\left(f^{n}, f^{t}\right)$



## Comparison with simulations

Cavity method

P. Wang et al. Physica A (2010)


Solution-no solution transition at $\mathrm{Z}_{\mathrm{c}}$

$$
\mathcal{Q}\left(\mathrm{Q}^{\rightarrow}\right)=\frac{1}{\mathcal{Z}} \sum_{z} z \mathrm{R}(z) \int \Omega\left(\left\{\hat{n}_{j}\right\}\right) \prod_{j=1}^{z-1} \mathrm{~d} \hat{n}_{j} \mathrm{DQ}^{\rightarrow j} \mathcal{Q}\left(\mathrm{Q}^{\rightarrow j}\right) \delta\left[\mathrm{Q}^{\left.\rightarrow-\mathcal{F}_{\rightarrow}\left(\left\{\mathrm{Q}^{\rightarrow j}\right\}\right)\right]}\right.
$$

## Comparison with simulations

Cavity method


Silbert et al. PRE (2002)


Consistent with interpretation of $z_{c}(\mu)$ as a lower bound

## Definition of jammed state: isostatic condition on $Z$


$z=$ geometrical coordination number. Determined by the geometry of the packing.

$$
Z \leq z \leq 2 d=6
$$

$Z=$ mechanical coordination number.
Determined by force/torque balance.

$$
\underset{\mu=\infty}{4=d}+1 \leq Z \leq 2 d=6
$$

## Generalizing the theory of monodisperse sphere packings

## Theory of monodisperse spheres

Polydisperse (binary) spheres

## Non-spherical objects

(dimers, triangles, tetrahedrons, spherocylinders, ellipses, ellipsoids ... )


Distribution of radius $P(r)$
 Extra degree of freedom

Onsager 1949

## Result of binary packings

Binary packings

$$
W=\frac{\pi}{2} \sum_{i=1}^{2} x_{i} \int_{0}^{\infty} c^{2} \exp \left\{\sum_{j}\left[-\rho_{i j}^{s}(z, x) S_{i j}^{*}(c)-\rho_{j}(W) V_{i j}^{*}(c)\right]\right\} d c
$$




Danisch, Jin, Makse, PRE (2010)

## The partition function for hard spheres

Volume Ensemble + Force Ensemble

1. The Volume Function: W (geometry)

2. Definition of jammed state: force and torque balance

Solution under different degrees of approximations

## Jammed packings in infinite dimensions


(b)

(c)
$\left(f(0), f\left(\frac{1}{2 w}\right), f\left(\frac{2}{2 w}\right), \cdots, f\left(\frac{n-1}{2 w}\right)\right)$

## Sloane <br> Most efficient design of signals <br> (Information theory)

Signal

## Sphere packings in high dimensions

Sloane


Rigorous bounds
Minkowsky lower bound: $\phi \sim 2^{-d}$
Kabatiansky-Levenshtein upper bound: $\phi \sim 2^{-0.5990 \ldots d}$
Question: what's the density of RCP in high dimensions?

## Determination of a lower bound on

 average coordination number $\bar{z}_{c}^{\min }(\mu)$

