Assembly of particle equilibria on a sphere

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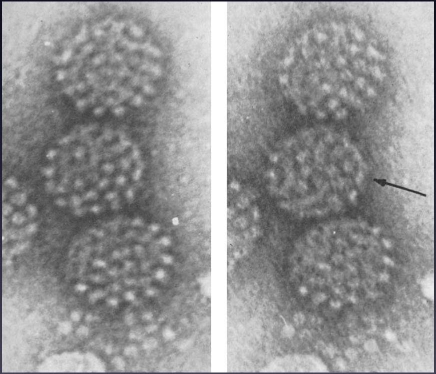
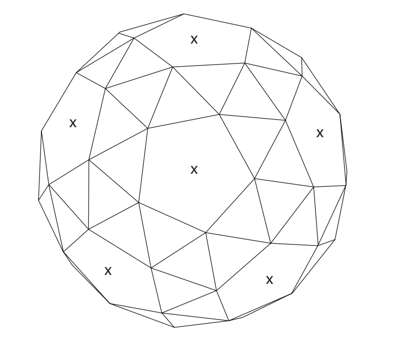
$N = 72$: Human polyoma virus (icosahedral symmetry)

X-ray diffraction imaging

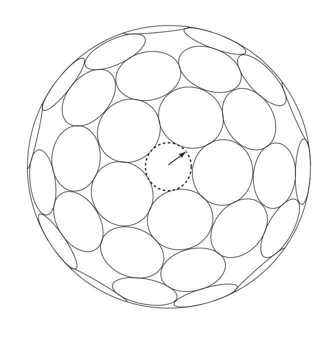


Klug & Finch (1965)

Snub dodecahedral ($N = 60$) structure

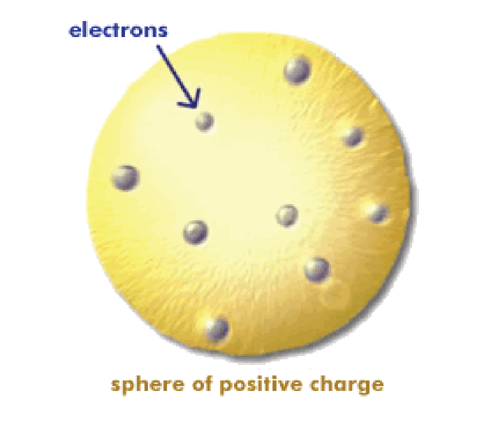


Can we get to $N = 72$?



Is it a 'best' packing?

J.J Thomson's plum-pudding model of the atom (1904)



An open problem[1] in constrained optimization

- Find extremizers for the Riesz-s energy E_s:

$$E_s = \sum_{i=1}^{N} \sum_{j=1}^{N}{}' |x_i - x_j|^{-s}, \quad s > 0$$

- ∇E_s is the 'interaction-energy' of the particle system
- $s \rightarrow 0$: E_0 logarithmic (point vortex)
- $s = 1$: E_1 Coulomb
- $s \rightarrow \infty$: Spherical packing problem (Tammes)
- Euler constraint: $F - E + V = 2$

[1] Proofs of global minimum or best packing only for $N = 2 - 12$ and $N = 24$

The interesting issues

- Structure of equilibria
- Growth/Formation/Assembly
- Stability/Robustness
- Control/Intervention

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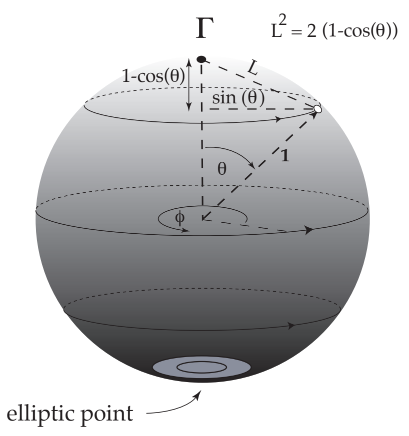
Outline

A charged particle



Spherical coordinates

- Field has no azimuthal dependence.
- Strength drops off monotonically with distance.

$$\dot{\theta} = 0$$

$$\dot{\phi} = \frac{\Gamma}{2\pi L^2} = \frac{\Gamma}{4\pi(1 - \cos\theta)}$$

Cartesian coordinates

$$\dot{\vec{x}} = \frac{\Gamma_\beta}{4\pi} \frac{\vec{x}_\beta \times \vec{x}}{(1 - \vec{x} \cdot \vec{x}_\beta)}$$

$$\vec{x}_\beta = (0, 0, 1); \quad \|\vec{x}\| = 1$$

$$\vec{x} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

- Linear superposition:

$$\dot{\vec{x}} = \sum_{\beta=1}^{N} \frac{\Gamma_\beta}{4\pi} \frac{\vec{x}_\beta \times \vec{x}}{(1 - \vec{x} \cdot \vec{x}_\beta)} \qquad \Gamma_\beta \in \mathbb{R}$$

- Each particle moves with the local velocity it feels due to all the others:

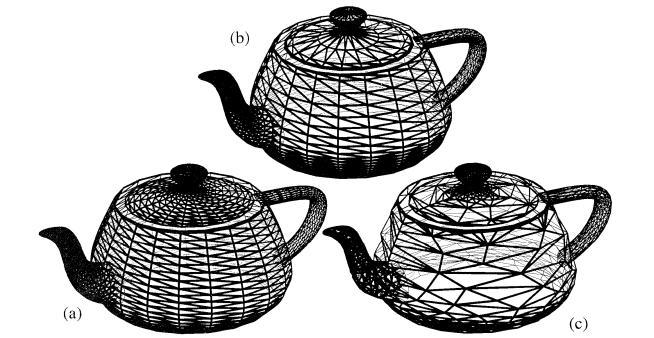
$$\dot{\vec{x}}_\alpha = {\sum_{\beta=1}^{N}}' \frac{\Gamma_\beta}{4\pi} \frac{\vec{x}_\beta \times \vec{x}_\alpha}{(1 - \vec{x}_\alpha \cdot \vec{x}_\beta)} \quad (\alpha = 1, ..., N)$$

The interacting particle system on a surface

$$\dot{\vec{x}}_\alpha = \sum_{\beta=1}^{N}{}' \frac{\Gamma_\beta}{4\pi} \frac{\hat{n}_\beta \times (\vec{x}_\alpha - \vec{x}_\beta)}{l_{\alpha\beta}^2}$$

$$l_{\alpha\beta}^2 = |\vec{x}_\alpha - \vec{x}_\beta|^2 = 2(1 - \vec{x}_\alpha \cdot \vec{x}_\beta)$$

The Utah teapot (Chouraqui & Elber 1996)



(a) Uniform sampling; (b) Spring-mass relaxation; (c) Charged particle equilibria

The Hamiltonian system

$$\mathcal{H} = -\frac{1}{4\pi} \sum_{\alpha<\beta} \Gamma_\alpha \Gamma_\beta \log(l_{\alpha\beta}^2)$$

$$P_\alpha \equiv \sqrt{|\Gamma_\alpha|}\cos(\theta_\alpha); \quad Q_\alpha \equiv \sqrt{|\Gamma_\alpha|}\phi_\alpha$$

$$\dot{P}_\alpha = \frac{\partial \mathcal{H}}{\partial Q_\alpha}, \quad \dot{Q}_\alpha = -\frac{\partial \mathcal{H}}{\partial P_\alpha}$$

Other conserved quantities

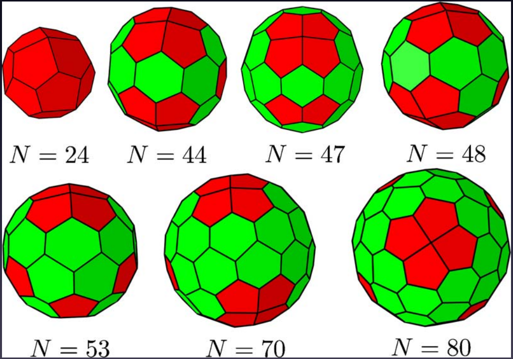
$$\vec{J} \equiv (J_x, J_y, J_z)$$

$$J_x = \sum_{\alpha=1}^{N} \Gamma_\alpha x_\alpha = \sum_{\alpha=1}^{N} \Gamma_\alpha \sin(\theta_\alpha)\cos(\phi_\alpha)$$

$$J_y = \sum_{\alpha=1}^{N} \Gamma_\alpha y_\alpha = \sum_{\alpha=1}^{N} \Gamma_\alpha \sin(\theta_\alpha)\sin(\phi_\alpha)$$

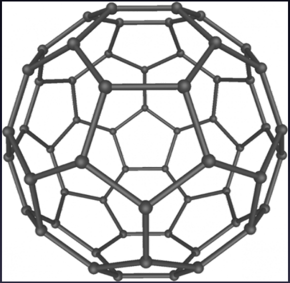
$$J_z = \sum_{\alpha=1}^{N} \Gamma_\alpha z_\alpha = \sum_{\alpha=1}^{N} \Gamma_\alpha \cos(\theta_\alpha)$$

Wales & Ulker (2006)



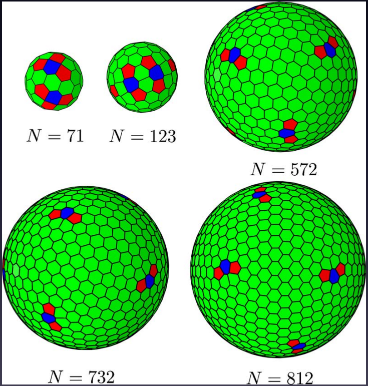
Red: pentagons Green: hexagons

Buckyball: $N = 60$



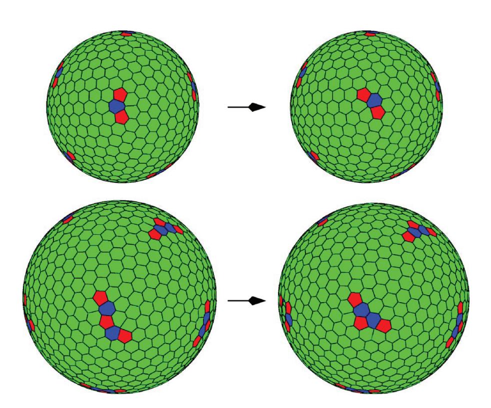
- C_{60} carbon molecule (Curl, Kroto, Smalley (1985))
- Truncated icosahedral structure
- 20 hexagons, 12 pentagons
- No two pentagons share an edge

Defects: 'scars'



Blue: septagons

Very delicate dynamics: migration over 'barriers'



Evolution through 'transition' states

Variational formulation

Variational approach has worked well for:

- Relatively small N and homogeneous particles
- Patterns exhibiting discrete symmetries
- Stable patterns

But not well for:

- Large N and mixed populations of particles
- Patterns with defects and asymmetries
- Unstable patterns, issues of assembly and formation

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Equilibria as fixed points: $l_{\alpha\gamma}^2 \equiv \|\vec{x}_\alpha - \vec{x}_\gamma\|^2$

The fixed point equation

$$\frac{d}{dt}(l_{\alpha\gamma}^2) = \sum_{\beta=1}^{N}{}'' \Gamma_\beta V_{\alpha\beta\gamma} \left[\frac{1}{l_{\beta\alpha}^2} - \frac{1}{l_{\beta\gamma}^2} \right] = 0$$

- Evolution equation for each line segment connecting pairs.
- $V_{\alpha\beta\gamma}$ is the volume subtended by the points $\mathbf{x}_\alpha$, $\mathbf{x}_\beta$, $\mathbf{x}_\gamma$.

The configuration matrix

$$A\vec{\Gamma} = 0, \quad A \in R^{M \times N}$$

$$M = \binom{N}{2} \quad \vec{\Gamma} \in R^N$$

$$AA^T \neq A^T A \quad \text{(non-normal)}$$

- Entries of A are the terms: $\Gamma_\beta V_{\alpha\beta\gamma} \left[\frac{1}{l_{\beta\alpha}^2} - \frac{1}{l_{\beta\gamma}^2} \right]$

Existence of relative equilibria

$$\det(A^T A) = 0$$

$$\mathrm{Rank}(A) < N$$

Uniqueness

$$\text{Nullspace}(A) = 1$$

$$\text{Rank}(A) = N - 1$$

Classification of equilibria via SVD

$$A^T A\vec{v}^{(i)} = (\sigma^{(i)})^2\vec{v}^{(i)} \qquad AA^T\vec{u}^{(i)} = (\sigma^{(i)})^2\vec{u}^{(i)}$$

$$\sigma^{(1)} \geq \ldots \geq \sigma^{(k)} > 0 \quad \textit{rank}$$

$$\sigma^{(k+1)} = \ldots = \sigma^{(N)} = 0 \quad \textit{nullspace}$$

$$\vec{v}^{(i)} = \vec{\Gamma}^{(i)}, \quad (i = k+1, \ldots, N) \quad \textit{basis}$$

Splitting of spectrum

$N - k =$ Nullspace (A) *Degeneracy*

$k =$ Rank (A)

- Is $\vec{\Gamma} = (1, 1, \ldots, 1) \in \text{Nullspace}(A)$?

Rank(A)

- Normalized eigenvalues of the covariance matrix $A^T A$:

$$\hat{\lambda}^{(i)} = \lambda^{(i)} / \sum_{j=1}^{k} \lambda^{(j)}$$

  can be interpreted as probabilities $P_i = \hat{\lambda}^{(i)}$
- The set of numbers P_i ($i = 1, ..., k$) can be thought of as a *discrete distribution* that characterizes the pattern

Spectral signature of the pattern

Shannon entropy

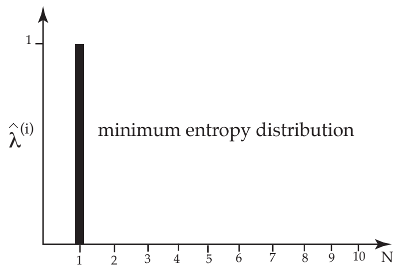
$$H = -\sum_{i=1}^{k} P_i \ln P_i \qquad (0 \leq H \leq \ln k)$$

Measures how sharply the spectrum drops off from max to min.

Minimum entropy

- If the distribution clustered in one state:

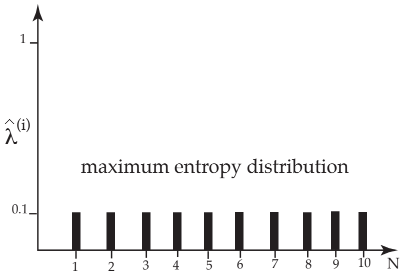
$$
\begin{aligned}
P_1 &= 1; \quad P_i = 0 \quad (i > 1) \\
H &= 0
\end{aligned}
$$



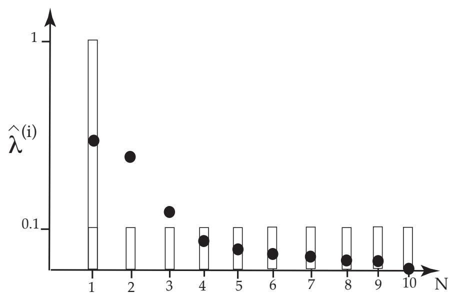
Maximum entropy

- Equal probabilities:

$$P_i = \frac{1}{N} \quad (i = 1, ..., N)$$
$$H = \ln N$$

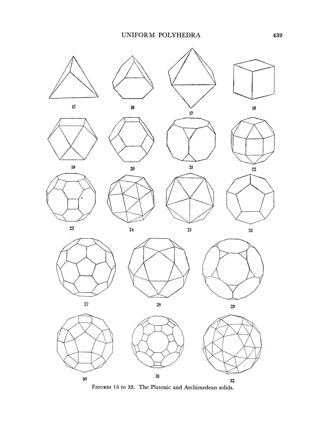


Typical distribution



- Distributions that drop-off sharply from the maximum are *lower* entropy configurations than those that are relatively flat around the maximum.

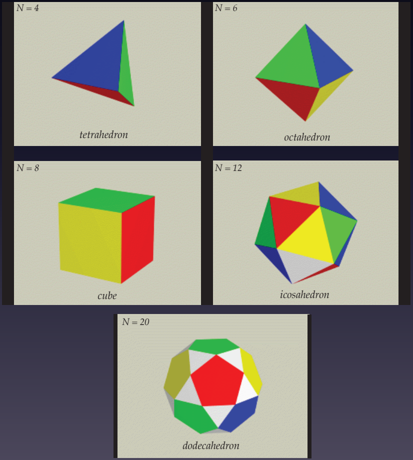
The 5 Platonic and 13 Archimedean solids

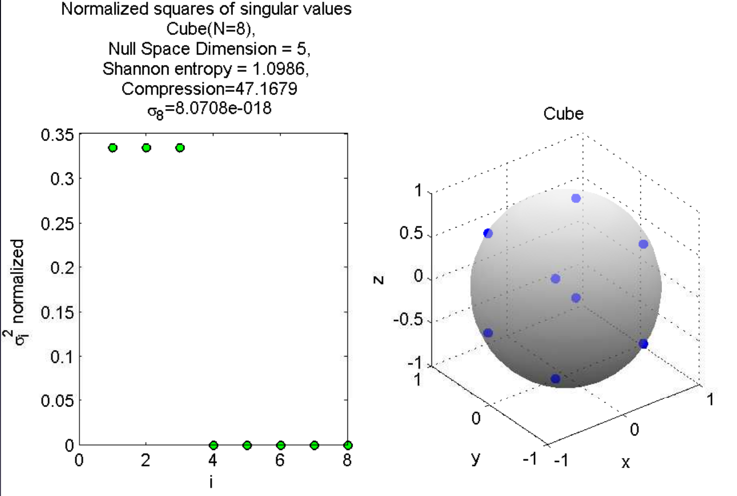


FIGURES 15 to 32. The Platonic and Archimedean solids.

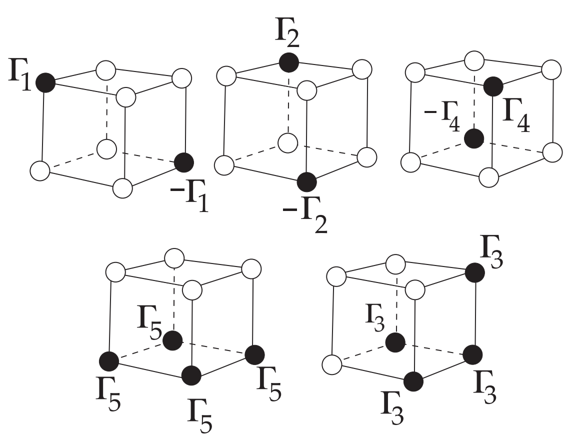
Coxeter classification

The 5 Platonic solids

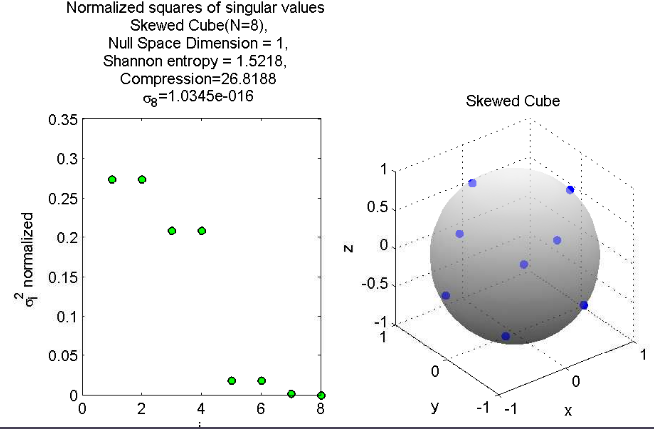



Normalized squares of singular values
Cube(N=8),
Null Space Dimension = 5,
Shannon entropy = 1.0986,
Compression=47.1679
σ8=8.0708e-018
σi2 normalized
i
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
2
4
6
8
Cube
z
x
y
1
0.5
0
-0.5
-1
1
0
-1
-1
0
1

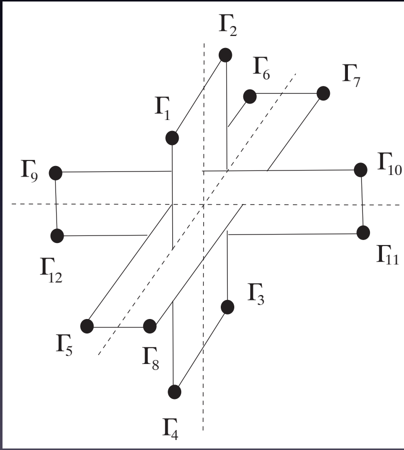
Nullspace = 5

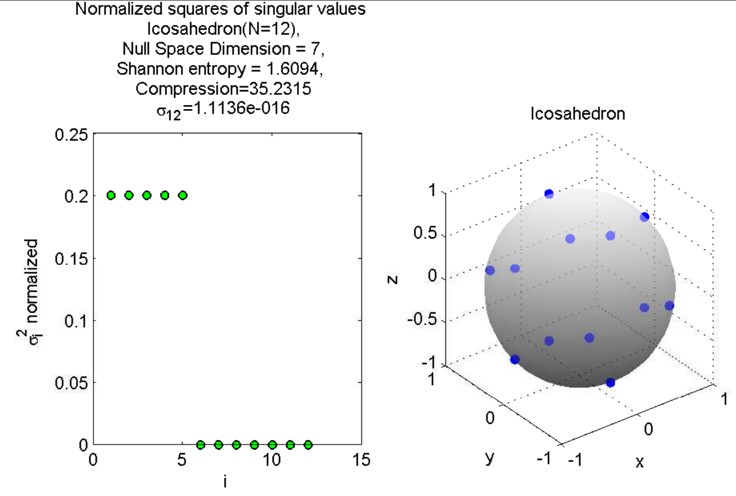

Γ_1
$-\Gamma_1$
Γ_2
$-\Gamma_2$
$-\Gamma_4$
Γ_4
Γ_5
Γ_5
Γ_5
Γ_5
Γ_3
Γ_3
Γ_3
Γ_3

Skewed cube: higher entropy, lower energy

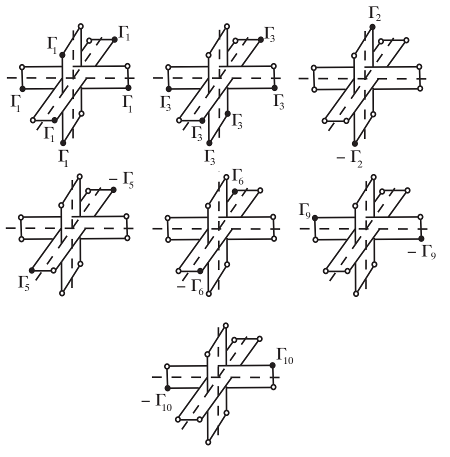


$N = 12$: Icosahedron

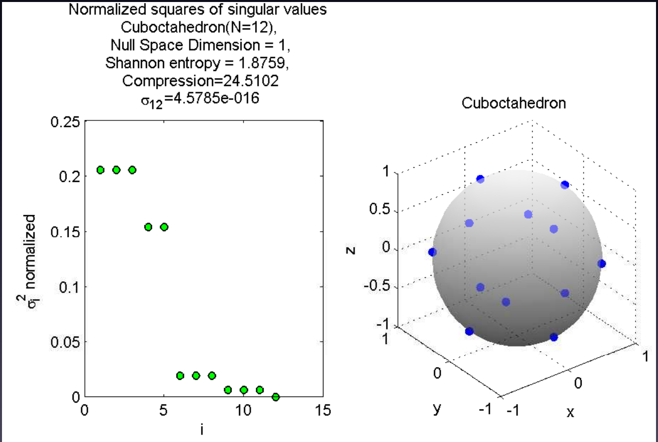



Normalized squares of singular values
Icosahedron(N=12),
Null Space Dimension = 7,
Shannon entropy = 1.6094,
Compression=35.2315
σ12=1.1136e-016
σi2 normalized
i
0.25
0.2
0.15
0.1
0.05
0
0
5
10
15
Icosahedron
z
y
x
1
0.5
0
-0.5
-1
1
0
-1
-1
0
1

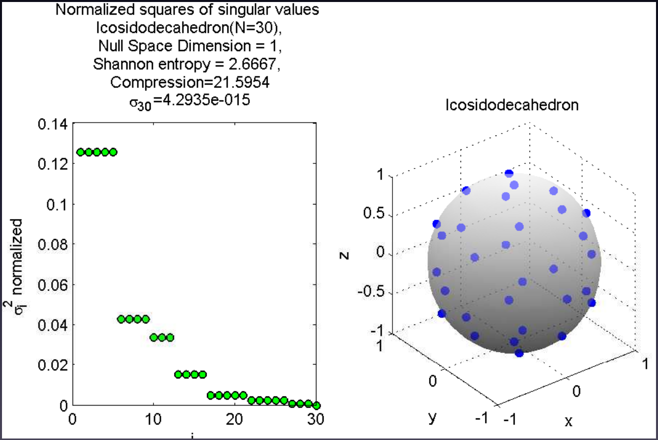
Nullspace = 7


Γ_1
Γ_1
Γ_1
Γ_1
Γ_1
Γ_1
Γ_3
Γ_3
Γ_3
Γ_3
Γ_3
Γ_3
Γ_2
$-\Gamma_2$
$-\Gamma_5$
Γ_5
Γ_6
$-\Gamma_6$
Γ_9
$-\Gamma_9$
Γ_{10}
$-\Gamma_{10}$

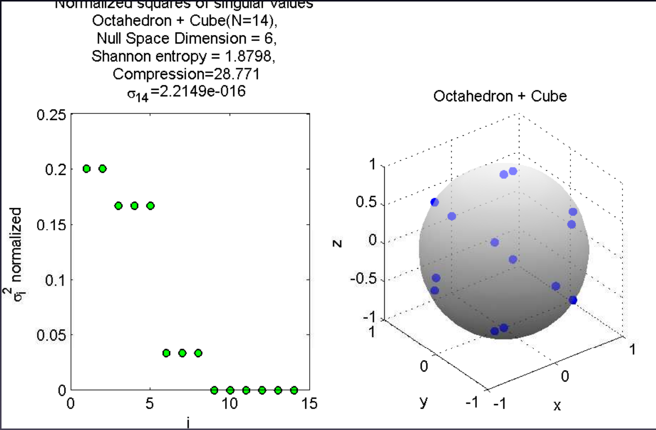
Archimedean: Cuboctahedron



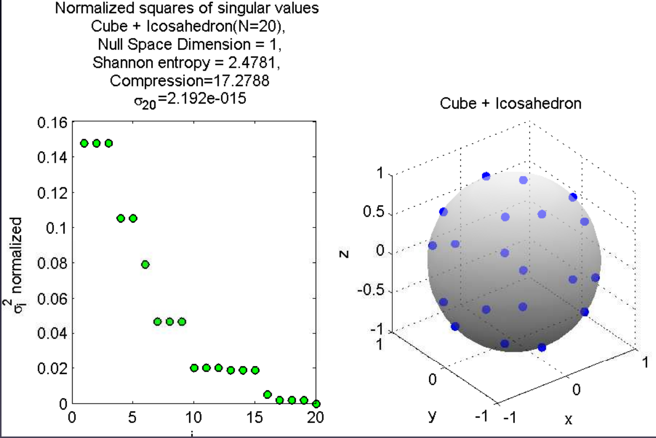
Archimedean: Icosidodecahedron



Superpositions: Cube + Octahedron

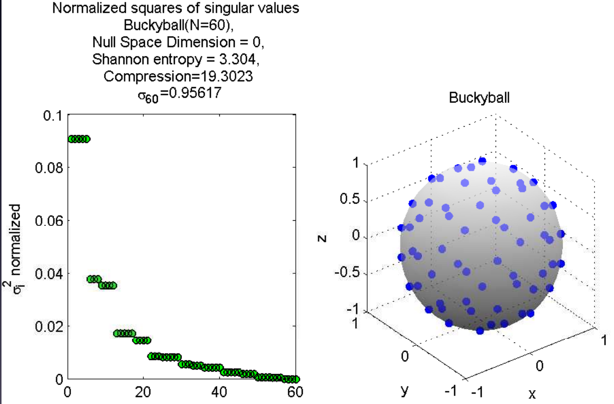


Superpositions: Cube + Icosahedron



Buckyball

Not all configurations have nontrivial nullspaces



Ingredients for ‘self-assembly’

- Systems are Hamiltonian, hence won’t naturally evolve to an equilibrium for generic initial conditions
- Need some ‘self-assembly’ mechanism
- Random fluctuations
- Gradient flow

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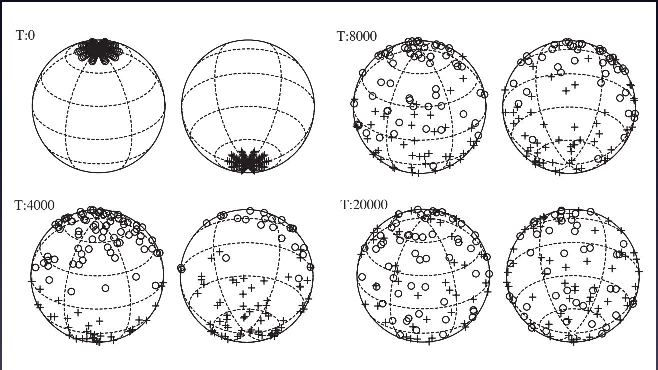
(i) The Brownian ratchet



Relies on random walk method on sphere and fast SVD solver

The ratchet scheme

- Randomly deposit N points on sphere
- Compute the singular values of A
- If smallest singular value is not below pre-determined convergence threshold, allow each particle to execute a random walk step (scaled with smallest singular value)
- Keep the new arrangement if the minimal singular value decreases from that of the previous step. Otherwise discard.
- Repeat
- When the smallest singular value drops below a pre-determined threshold, the algorithm has converged to an equilibrium

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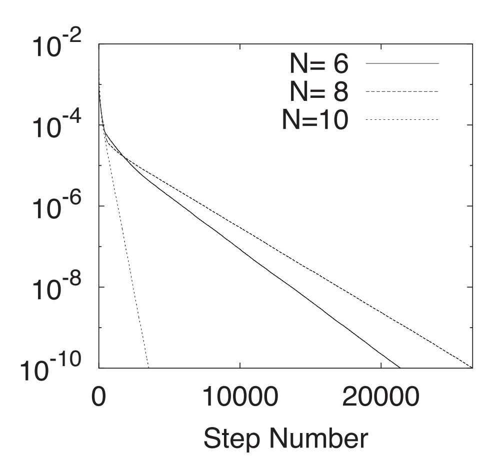
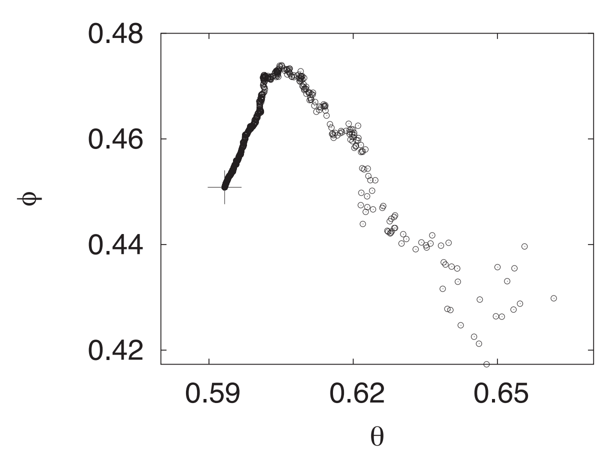
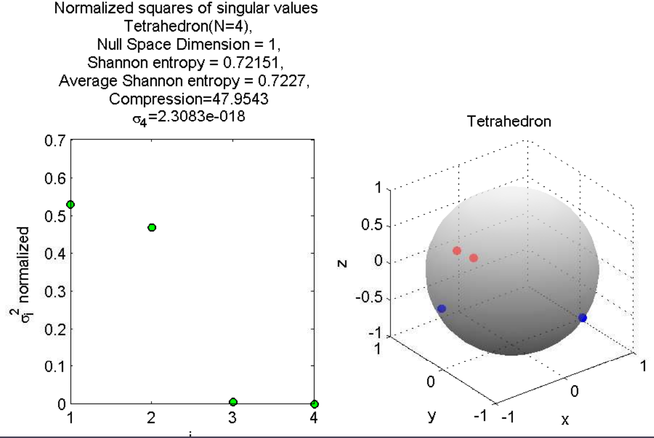
Convergence



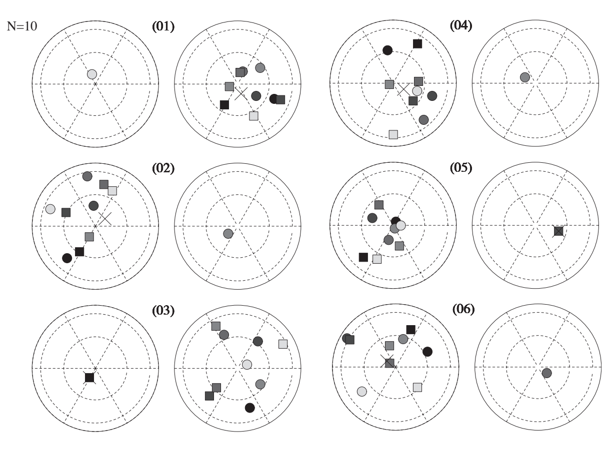
Random walk to final state



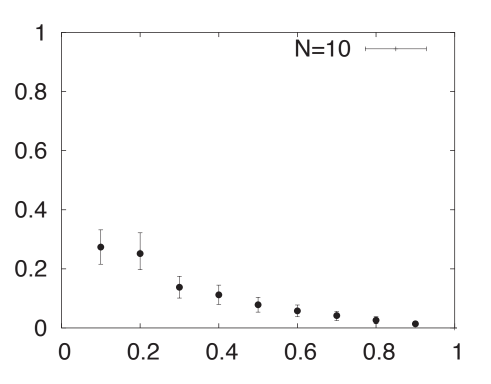
Constrained: ratchet a defect



Unconstrained: asymmetric equilibria



Ensemble averaged singular value distribution



Asymmetric equilibria, on average, have higher Shannon entropy than symmetric ones

(ii) Gradient flow

A. Barreiro, J. Bronski & P.K. Newton (2009)

Spectral gradient flow

$$A_t = -\nabla_A \det(A^T A)$$

unconstrained: $A\vec{\Gamma} = 0$

constrained: $\vec{\Gamma} = (1, \ldots, 1)$

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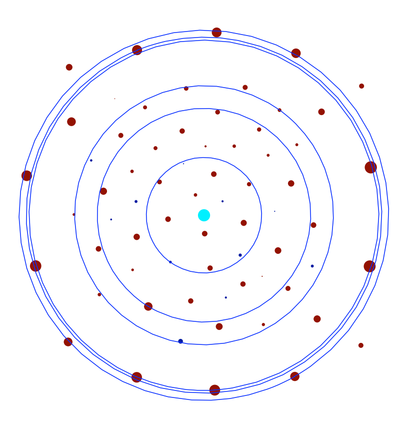
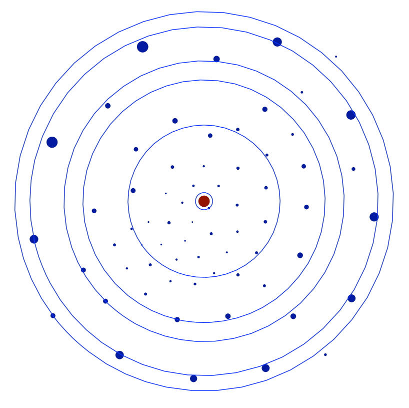
Unconstrained



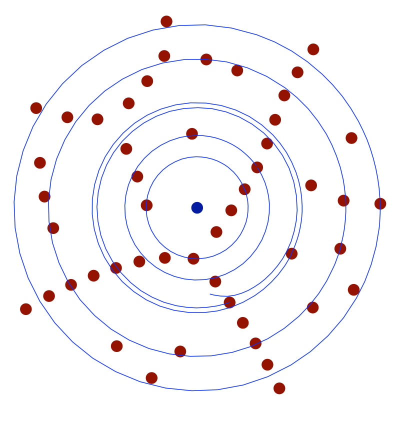
$N = 67$

Unconstrained



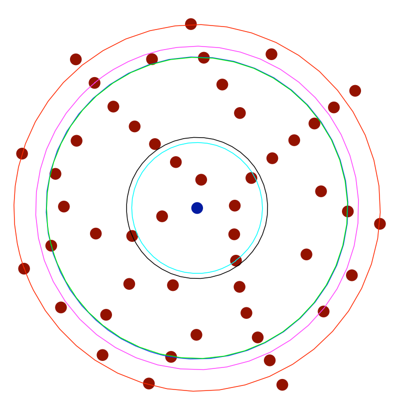
$N = 67$

Constrained



$N = 50$

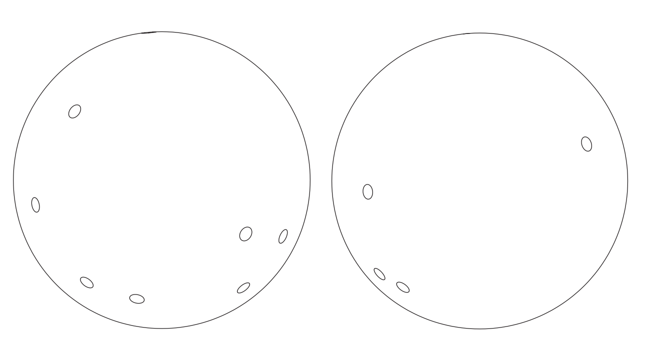
Constrained



$N = 50$

(iii) Yin-Yang scheme (Longuet-Higgins (2009))

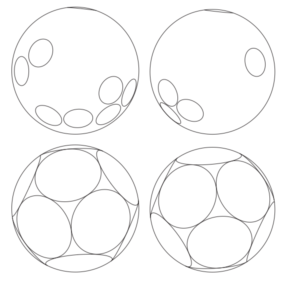
Yin: Randomly perturb each center, calculate θ_{min}



Random placement of 12 equal circles on the sphere

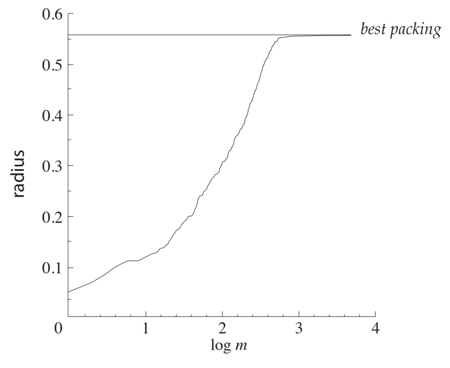
Yang: $\delta^* \rightarrow \delta + F \cdot \left(\frac{1}{2}\theta_{min} - \delta\right)$

Convergence to icosahedron



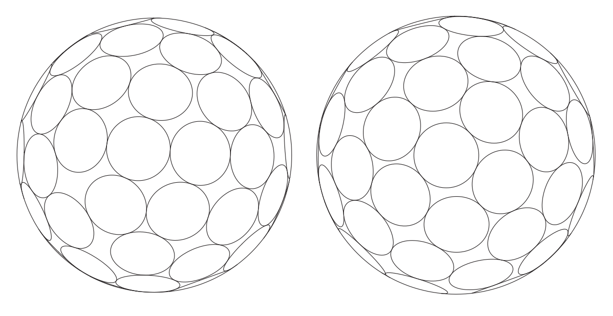
- δ is dimensionless ratio of cap-radius to sphere-radius
- 'Yang' step can be thought of as 'shrinking' the sphere (outer protein sheath) instead of growing δ

$\delta = \arcsin(\tau + 2)^{-1/2} = 0.55357$



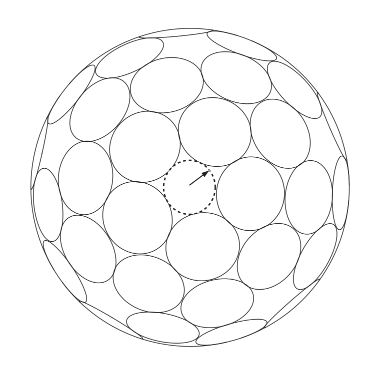
Best packing for $N = 12$ AND nullspace = 7

For $N = 60$, snub dodecahedron is not the best packing and has empty nullspace

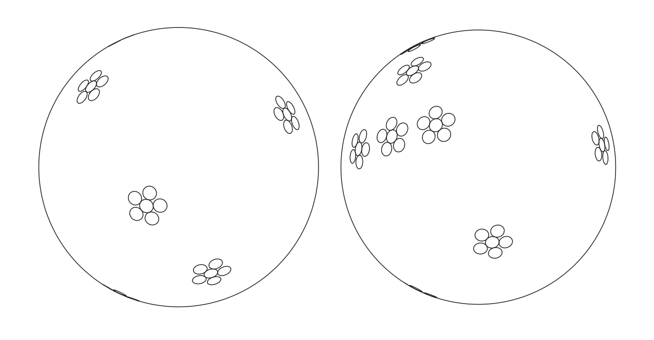


Less symmetric arrangement gives better packing

For $N = 72$, method generally does not converge to snub dodecahedron + 12

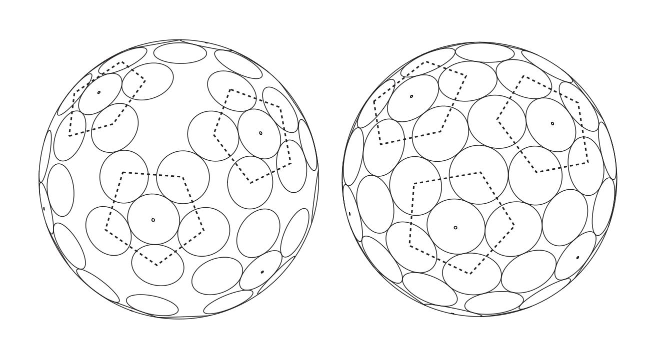


How to get there? ‘Multi-stage assembly’ + Yin-Yang



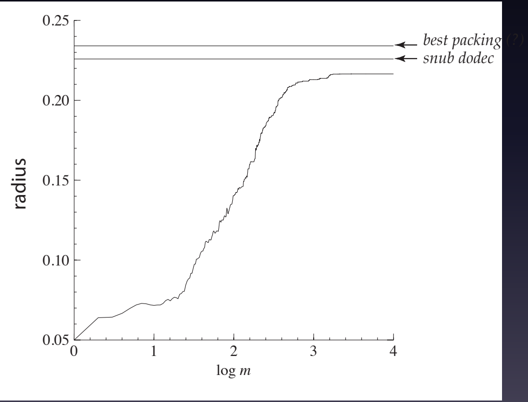
Growth: Flower petal structure (12×6)

Convergence



60 units surrounded by 6   12 units surrounded by 5

Packing not as tight as snub dodecahedron



Longuet-Higgins (2009)

Stability theory

- Just starting! (Vitalii Ostrovskyi - USC Math)
- Based on

$$\mathcal{H} = -\frac{1}{4\pi}\sum_{\alpha<\beta}\Gamma_\alpha\Gamma_\beta \log(l_{\alpha\beta}^2); \quad \vec{J} = \text{const.}$$

- And on expansion of fixed point system:

$$\frac{d}{dt}(\vec{l_0} + \epsilon\vec{l_1} + \ldots) = (A_0 + \epsilon A_1 + \ldots)\vec{\Gamma}$$

$$\frac{d}{dt}(\vec{l_0}) = A_0\vec{\Gamma} = 0; \quad \frac{d}{dt}(\vec{l_1}) = A_1\vec{\Gamma}$$

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Summary

- Equilibria as fixed points instead of extremizers
- Spectral decomposition of the configuration matrix
  - Degeneracy (nullspace)
  - Entropy
- Numerical schemes that also model physics
  - Brownian ratchet schemes
  - Spectral gradient schemes
  - Yin-Yang + Multi-stage assembly

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