Assembly of particle equilibria on a sphere

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Equations of motion
The singular value spectrum of a configuration
Some examples: Coxeter polyhedra
Numerical schemes that ‘assemble’ the equilibria
Summary
References

Motivations
Particles on a sphere
Hamiltonian and other conserved quantities
Low $N \rightarrow$ High $N$

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

X-ray diffraction imaging

Klug & Finch (1965)

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Equilibria assembly on a sphere
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 \(E_s\):
  \[
  E_s = \sum_{i=1}^{N} \sum_{j=1}^{N} \left| x_i - x_j \right|^{-s}, \quad s > 0
  \]

- \(\nabla E_s\) is the ‘interaction-energy’ of the particle system
- \(s \to 0 : E_0\) logarithmic (point vortex)
- \(s = 1 : E_1\) Coulomb
- \(s \to \infty: \) 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

1. Equations of motion
   - Motivations
   - Particles on a sphere
   - Hamiltonian and other conserved quantities
   - Low $N \rightarrow$ High $N$

2. The singular value spectrum of a configuration
   - The fixed point equation
   - The configuration matrix approach
   - The singular value distribution

3. Some examples: Coxeter polyhedra

4. Numerical schemes that ‘assemble’ the equilibria
   - The Brownian ratchet scheme
   - Spectral gradient flow
   - Yin-Yang scheme
A charged particle

\[ L^2 = 2 \left(1 - \cos(\theta)\right) \]

elliptic point
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:

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

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

\[ \vec{\dot{x}}_{\alpha} = \sum_{\beta=1}^{N} \frac{\Gamma_{\beta}}{4\pi} \frac{\vec{x}_{\beta} \times \vec{x}_{\alpha}}{(1 - \vec{x}_{\alpha} \cdot \vec{x}_{\beta})} \quad (\alpha = 1, \ldots, N) \]
The interacting particle system on a surface

\[ \dot{\vec{x}}_\alpha = \sum_{\beta=1}^{N} \frac{\Gamma_\beta}{4\pi} \hat{n}_\beta \times \left( \vec{x}_\alpha - \vec{x}_\beta \right) \]

\[ l_{\alpha\beta}^2 = \left| \vec{x}_\alpha - \vec{x}_\beta \right|^2 = 2(1 - \vec{x}_\alpha \cdot \vec{x}_\beta) \]
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’

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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
Variational formulation

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Equilibria as fixed points: \[ l^2_{\alpha\gamma} \equiv \| \vec{x}_\alpha - \vec{x}_\gamma \|^2 \]

The fixed point equation

\[
\frac{d}{dt}(l^2_{\alpha\gamma}) = \sum_{\beta=1}^{N} \quad "\Gamma_\beta V_{\alpha\beta\gamma} \left[ \frac{1}{l^2_{\beta\alpha}} - \frac{1}{l^2_{\beta\gamma}} \right] = 0
\]

- Evolution equation for each line segment connecting pairs.
- \( V_{\alpha\beta\gamma} \) is the volume subtended by the points \( x_\alpha, x_\beta, x_\gamma \).
The configuration matrix

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

\[ M = \binom{N}{2} \quad \vec{\Gamma} \in \mathbb{R}^N \]

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

- Entries of \( A \) are the terms:

\[ \Gamma_{\beta} V_{\alpha\beta\gamma} \left[ \frac{1}{l^{2}_{\beta\alpha}} - \frac{1}{l^{2}_{\beta\gamma}} \right] \]
Existence of relative equilibria

\[ \det(A^T A) = 0 \]

\[ \text{Rank}(A) < N \]
Uniqueness

Nullspace(A) = 1

Rank(A) = N - 1
Classification of equilibria via SVD

\[ A^T A \bar{v}^{(i)} = (\sigma^{(i)})^2 \bar{v}^{(i)} \quad AA^T \bar{u}^{(i)} = (\sigma^{(i)})^2 \bar{u}^{(i)} \]

\[ \sigma^{(1)} \geq \ldots \geq \sigma^{(k)} > 0 \quad \text{rank} \]

\[ \sigma^{(k+1)} = \ldots = \sigma^{(N)} = 0 \quad \text{nullspace} \]

\[ \bar{v}^{(i)} = \bar{\Gamma}^{(i)}, \quad (i = k + 1, \ldots, N) \quad \text{basis} \]
Splitting of spectrum

\[ N - k = \text{Nullspace} \ (A) \]

**Degeneracy**

\[ k = \text{Rank} \ (A) \]

- 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 $P_i$ ($i = 1, \ldots, k$) can be thought of as a *discrete distribution* that characterizes the pattern
Spectral signature of the pattern

Shannon entropy

\[ H = - \sum_{i=1}^{k} P_i \ln P_i \quad (0 \leq H \leq \ln k) \]

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

- If the distribution clustered in one state:

\[ P_1 = 1; \quad P_i = 0 \quad (i > 1) \]

\[ H = 0 \]

Minimum entropy distribution
Maximum entropy

- Equal probabilities:

\[ P_i = \frac{1}{N} \quad (i = 1, \ldots, N) \]

\[ H = \ln N \]
• 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
The 5 Platonic solids

- **tetrahedron** (N = 4)
- **cube** (N = 6)
- **octahedron** (N = 8)
- **icosahedron** (N = 12)
- **dodecahedron** (N = 20)
Normalized squares of singular values

Cube (N=8),
Null Space Dimension = 5,
Shannon entropy = 1.0986,
Compression = 47.1679,
\( \sigma_2 = 8.0708 \times 10^{-18} \)
Nullspace = 5
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,
\( \sigma_{12} = 1.1136 \times 10^{-16} \)
Nullspace = 7

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Archimedean: Cuboctahedron

Normalized squares of singular values:
- Cuboctahedron (N=12), Null Space Dimension = 1, Shannon entropy = 1.8759, Compression=24.5102, \( \sigma_{12} \approx 4.5785 \times 10^{-016} \)

Graph showing normalized squares of singular values against index i.

3D plot of Cuboctahedron with points distributed on the sphere.

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Archimedean: Icosidodecahedron

Normalized squares of singular values
Icosidodecahedron (N=30),
Null Space Dimension = 1,
Shannon entropy = 2.6667,
Compression = 21.5954,
$\sigma_{30} = 4.2935 \times 10^{-15}$

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Superpositions: Cube + Octahedron

Normalized squares of singular values:
- Octahedron + Cube (N=14),
- Null Space Dimension = 6,
- Shannon entropy = 1.8798,
- Compression = 28.771,
- $\sigma_{14} = 2.2149 \times 10^{-16}$

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Only superposition of two or more solids with big nullity and small number of vortices gives rise of new equilibria. Also, there might be different equilibria depending on how we merge two solids. Example: superposition of octahedron and cube.

Figure 20: Octahedron + Cube
Superpositions: Cube + Icosahedron

Normalized squares of singular values
Cube + Icosahedron (N=20),
Null Space Dimension = 1,
Shannon entropy = 2.4781,
Compression = 17.2788
\( \sigma_{20} = 2.192 \times 10^{-15} \)
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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The ratchet scheme

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Convergence

![Graph showing convergence for different values of N]
Random walk to final state
Constrained: ratchet a defect

Normalized squares of singular values
Tetrahedron (N=4),
Null Space Dimension = 1,
Shannon entropy = 0.72151,
Average Shannon entropy = 0.7227,
Compression = 47.9543
\( \sigma_4 = 2.3083 \times 10^{-18} \)
Unconstrained: asymmetric equilibria

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Equilibria assembly on a sphere
Asymmetric equilibria, on average, have higher Shannon entropy than symmetric ones.
(ii) Gradient flow


**Spectral gradient flow**

\[ A_t = -\nabla_A \det(A^T A) \]

unconstrained: \( A\vec{r} = 0 \)
constrained: \( \vec{r} = (1, \ldots, 1) \)
(ii) Gradient flow


Spectral gradient flow

\[ A_t = -\nabla_A \det(A^T A) \]

unconstrained: \( A\vec{\Gamma} = 0 \)

constrained: \( \vec{\Gamma} = (1, ..., 1) \)
(ii) Gradient flow


Spectral gradient flow

\[ A_t = -\nabla_A \det(A^T A) \]

unconstrained: \( A\vec{\Gamma} = 0 \)

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

$N = 67$
Unconstrained

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The Brownian ratchet scheme
Spectral gradient flow
Yin-Yang scheme

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Equilibria assembly on a sphere

\[ N = 67 \]
Constrained

$N = 50$
Constrained

$N = 50$
(iii) Yin-Yang scheme (Longuet-Higgins (2009))

**Yin**: Randomly perturb each center, calculate $\theta_{\text{min}}$

Random placement of 12 equal circles on the sphere
Yang: $\delta^* \rightarrow \delta + F \cdot \left(\frac{1}{2} \theta_{\text{min}} - \delta\right)$

Convergence to icosahedron

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

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

• And on expansion of fixed point system:

\[
\begin{align*}
\frac{d}{dt}(l_0 + \epsilon l_1 + \ldots) &= (A_0 + \epsilon A_1 + \ldots)\vec{\Gamma} \\
\frac{d}{dt}(l_0) &= A_0 \vec{\Gamma} = 0;
\end{align*}
\]

\[
\frac{d}{dt}(l_1) = A_1 \vec{\Gamma}
\]
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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