Vortex lattice theory

A particle interaction perspective

P.K. Newton

Viterbi School of Engineering
&
Department of Mathematics
University of Southern California
Recent experiments in Bose-Einstein condensates

Interacting particle formulation
- Hamiltonian formulation
- Kelvin's variational principle
- Shift from stable pattern classification to nonequilibrium dynamics

The configuration matrix approach
- Lattices as fixed points
- Singular value distribution
- Pattern decomposition
- Shannon entropy of a lattice

Brownian ratchet schemes

Overview of related problems

References
Maxwell (1861)

Magnetic field lattice with ‘idle wheel’ particles carrying electric current
Direct imaging of Abrikosov lattices: (1967 - 1989)

**Left:** Type II superconductor (Essmann & Trauble 1967)

**Right:** $NbSe_2$ lattice using a scanning-tunneling microscope (Hess et al. 1989)
BEC’s: Ketterle (2001)

Vortex lattices in Bose-Einstein condensates with 16, 32, 80, and 130 vortices
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

BEC’s: Cornell (2002)

Front view and side view of a regular BEC lattice showing 2D structure with nearly parallel filaments

FIG. 1. (a) Expansion picture of a vortex lattice seen along the rotation axis. (b) One pixel wide cross section along the white line in (a). (c) Expansion picture of a different condensate rotating more slowly than in (a), seen from the side.

FIG. 2. Lattice evolution after an $m_z = -2$ excitation. Pictures taken (a) 173 ms and (b) 873 ms after start of trap deformation.

FIG. 3. Change of lattice structure. (a) Hexagonal structure in an undisturbed lattice. (b) Near orthorhombic structure seen transiently during lattice evolution in the presence of an $m_z = -2$ quadrupolar surface mode.

FIG. 4. (a) Sheet-like structure as seen during lattice evolution in the presence of an $m_z = -2$ quadrupolar surface mode. (b) Cross section integrated over the white box in (a). Even though the box is wider than the calculated vortex core spacing, the observed contrast is nearly perfect. (c-e) Same as (a), but observed in a more deformed trap with $\{\omega_x,\omega_y,\omega_z\} = 2\pi \{6.0, 8.6, 13.8\}$ Hz.

FIG. 5. (a-e) Nondestructive in-trap images of the sheet-like structures seen along the x-direction [conditions similar to Fig. 4(a)]. Spacing between images 10.6 ms. Note the very different spatial scale from expansion images (e.g., Fig. 1). (f) Cross section of (a), integrated over the condensate.
Magnetically confined non-neutral plasmas

Lattices with $N = 3, 5, 7, 9, 6$ - the vortices are magnetically confined pure electron columns

Fine et al. (1995)
Floating magnetic rotating discs on fluid air interface

Configurations for $N = 10, 12, 19$ are not unique and patterns can oscillate between the two

Grzybowski et al. (2000)
Mayer’s magnets (1878)

\[ N = 1 - 8 \]

Derr – Floating Magnets.

Derr (1909)
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

\[ N = 1 \rightarrow 52 \]

Derr (1909)

P.K. Newton  Vortex lattice theory
Why a particle model?

(i) Core region \((r \to 0)\)  
(ii) Monotonic decay \((r \to \infty)\)

Abrikosov (1957)
The particle model

\[
\dot{z}^* = \frac{\Gamma}{2\pi i} \frac{1}{z}
\]
velocity field due to vortex at origin

\[
u_r = \dot{r} = 0 \quad \text{circumferential}
\]

\[
u_\theta = r\dot{\theta} = \frac{\Gamma}{2\pi r} \quad \text{drops off linearly}
\]

\[
\dot{z}^* = \frac{\Gamma_\beta}{2\pi i} \cdot \frac{1}{z - z_\beta}
\]
point vortex at \(z_\beta\)
The particle model

\[ \dot{z}^* = \frac{1}{2\pi i} \sum_{\beta=1}^{N} \frac{\Gamma_\beta}{z - z_\beta} \]

contributions from each site

\( N \)-vortex equations

\[ \dot{z}_\alpha^* = \frac{1}{2\pi i} \sum_{\beta=1}^{N} \frac{\Gamma_\beta}{z_\alpha - z_\beta} \]

Helmholtz II (1858)
The particle model

Discrete Biot-Savart law

\[ \dot{\vec{x}}_\alpha = \sum_{\beta=1}^{N} \frac{\Gamma_\beta}{2\pi} \cdot \frac{\hat{n}_\beta \times (\vec{x}_\alpha - \vec{x}_\beta)}{||\vec{x}_\alpha - \vec{x}_\beta||^2} \]

\[ \vec{x}_\alpha \equiv (x_\alpha(t), y_\alpha(t)) \equiv x_\alpha + iy_\alpha = z_\alpha(t) \]

\[ \hat{n}_\beta = \hat{e}_z \quad \text{planar flow} \]

\[ = \vec{x}_\beta / R, \quad ||\vec{x}_\beta|| = R, \quad \text{sphere} \]

\[ l_{\alpha\beta}^2 \equiv ||\vec{x}_\alpha - \vec{x}_\beta||^2 \quad \text{ intervortical distances} \]
The particle model

Statement of problem

(i) Given a set of \( N \) points in the complex plane \( z_\alpha(0) \in \mathbb{C} \), \( \alpha = 1, \ldots, N \), find the set of vortex strengths \( \vec{\Gamma} = (\Gamma_1, \Gamma_2, \ldots, \Gamma_N) \in \mathbb{R}^N \) so that all intervortical distances \( l^2_{\alpha\beta} = |z_\alpha - z_\beta|^2, (\alpha \neq \beta) \) remain fixed. In particular, find a basis set for this subspace of \( \mathbb{R}^N \).

(ii) For a given set of vortex strengths \( \vec{\Gamma} \in \mathbb{R}^N \), find the set of points \( z_\alpha(0) \in \mathbb{C}, \alpha = 1, \ldots, N \) so that all intervortical distances remain fixed.
Hamiltonian formulation

Logarithmic interaction

\[
\Gamma_\alpha \dot{x}_\alpha = \frac{\partial H}{\partial y_\alpha}; \quad \Gamma_\alpha \dot{y}_\alpha = -\frac{\partial H}{\partial x_\alpha}
\]

\[
H = -\frac{1}{4\pi} \sum_{\beta=1}^{N} \sum_{\alpha=1}^{N} \Gamma_\alpha \Gamma_\beta \ln |z_\alpha - z_\beta|
\]

\[
X + iY = \sum_{\alpha=1}^{N} \Gamma_\alpha z_\alpha; \quad I = \sum_{\alpha=1}^{N} \Gamma_\alpha |z_\alpha|^2
\]
Kelvin’s variational principle

Assume entire configuration moves as a rigid body:

$$\dot{z}_\alpha = V + i\omega z_\alpha \quad \text{ansatz}$$

$$V^* - i\omega z^*_\alpha = \frac{1}{2\pi i} \sum_{\beta=1}^{N} i \Gamma_\beta z_\alpha - z_\beta, \quad (\alpha = 1, \ldots, N).$$
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Kelvin’s variational principle

Constrained Lagrange multiplier method

Extremize the augmented Hamiltonian

\[ \mathcal{H} + V \sum_{\alpha=1}^{N} \Gamma_{\alpha} x_{\alpha} - u \sum_{\alpha=1}^{N} \Gamma_{\alpha} y_{\alpha} + \frac{1}{2} \omega \sum_{\alpha=1}^{N} \Gamma_{\alpha} |z_{\alpha}|^2 \]

\[ V = u + iv \] and \( \omega \) play the role of Lagrange multipliers
Constraints - conservation of linear impulse
\( X + iY = \sum_{\alpha=1}^{N} \Gamma_{\alpha} z_{\alpha} \) and angular impulse \( I = \sum_{\alpha=1}^{N} \Gamma_{\alpha} |z_{\alpha}|^2 \)
Variational formulation has worked well for:

- Relatively small $N$
- $\Gamma_\beta = 1$
- Patterns exhibiting discrete symmetries
- Stable patterns
Stable regular polygonal lattices $N = 4, 5$

Gueron & Shafrir (1999)
Regular polygons in superfluid Helium

Yarmchuck et al. (1979)
Lowest energy state for \( N = 18 \)

Campbell & Ziff (1979)
Others at higher energies

Campbell & Ziff (1979)
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Hamiltonian formulation
Kelvin's variational principle
Shift from stable pattern classification to nonequilibrium dynamics

\[ N = 217 \]

Campbell & Ziff (1979)

P.K. Newton
Vortex lattice theory
Lattice under stress

---

**FIG. 1.** (a) Expansion picture of a vortex lattice seen along the rotation axis. (b) One pixel wide cross section along the white line in (a). (c) Expansion picture of a different condensate rotating more slowly than in (a), seen from the side.

**FIG. 2.** Lattice evolution after an $m_z = -2$ excitation. Pictures taken (a) 173 ms and (b) 873 ms after start of trap deformation.

**FIG. 3.** Change of lattice structure. (a) Hexagonal structure in an undisturbed lattice. (b) Near orthorhombic structure seen transiently during lattice evolution in the presence of an $m_z = -2$ quadrupolar surface mode.

**FIG. 4.** (a) Sheet-like structure as seen during lattice evolution in the presence of an $m_z = -2$ quadrupolar surface mode. (b) Cross section integrated over the white box in (a). Even though the box is wider than the calculated vortex core spacing, the observed contrast is nearly perfect. (c-e) Same as (a), but observed in a more deformed trap with $\{\omega_x, y, z\} = 2\pi \{6.0, 8.6, 13.8\}$ Hz.

**FIG. 5.** (a-e) Nondestructive in-trap images of the sheet-like structures seen along the x-direction [conditions similar to Fig. 4(a)]. Spacing between images 10.6 ms. Note the very different spatial scale from expansion images (e.g., Fig. 1). (f) Cross section of (a), integrated over the condensate.
Point and grain boundary defects

Ketterle et al. (2001)
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Tkachenko oscillations

Cornell et al. (2003)
Formation with random background

Fig. 1.14 Lattice formation is remarkably robust, as shown here for three successive times of a vortex-in-cell simulation from Jin and Dubin (2000) (reprinted with permission from APS) for five point vortices in a random background. Also plotted is the minimum distance between the point vortices, with the arrow showing the approximate “cooling time” at which the crystal structure sets in.

Fig. 1.15 Lattices with \( N = 3, 5, 7, 9, 6 \) formed in a magnetically confined nonneutral plasma, from Fine et al. (1995) (reprinted with permission from APS), which mimic some of the patterns produced in Campbell and Ziff (1978, 1979) as well as those shown in Figures 1.2 and 1.13. The vortices are magnetically confined pure electron columns. Note that the case \( N = 9 \) appears to have a stronger vortex at the center, surrounded by 8 equal strength vortices around the circular perimeter.

2. Interacting Particle Formulation. We begin with the assumption of a planar velocity field that has only radial dependence of the form

\[
\mathbf{u}(r) = \alpha r^{-1}.
\]

This is most conveniently written in complex variable notation:

\[
\dot{z}^* = \frac{\Gamma}{2\pi i} \frac{1}{z},
\]

(2.1)

Jin & Dubin (2000)
Reformation via random walk

Cornell et al. (2003)
Recent experiments in Bose-Einstein condensates

Asymmetric lattices

V. Bretin, Y. Castin, G. Shlyapnikov, and J. Dalibard, cond-mat/0201568.


Cornell et al. (2002)
Variational formulation has not worked well for:

- Large $N$
- Heterogeneous equilibria where $\Gamma_\beta$ not all equal
- Pattern defects
- Asymmetric equilibria
- Unstable patterns
- Formation dynamics in the presence of randomness (robustness)
- Far from equilibrium fluctuations
- Finding $\Gamma_\beta$ is NOT part of the theory- it must be assumed a priori
Fixed point approach

Interparticle distance equation

$$\frac{d}{dt} \left( l^2_{\alpha\lambda} \right) = \sum_{\beta=1}^{N} \Gamma_{\beta} A_{\alpha\lambda\beta} \left( \frac{1}{l^2_{\alpha\beta}} - \frac{1}{l^2_{\lambda\beta}} \right) \quad (\alpha, \lambda = 1, \ldots, N).$$

$A_{\alpha\lambda\beta}$ is the (signed) area subtended by the points $\vec{x}_\alpha$, $\vec{x}_\lambda$, $\vec{x}_\beta$.
Fixed point approach

Relative equilibria as fixed points

\[ \frac{d}{dt} \left( I^2_{\alpha\lambda} \right) = 0 \Rightarrow \]

\[ A \vec{\Gamma} = 0 \]

A has N columns and \( N(N - 1)/2 \) rows, and \( \vec{\Gamma} = (\Gamma_1, \Gamma_2, \ldots, \Gamma_N) \).
Fixed point approach

- The *configuration matrix* $A$ encodes the *geometry* of the pattern.
- Only those with non-trivial nullspaces produce lattices.
- The strength vector $\vec{\Gamma} \in \mathbb{R}^N$ is found a posteriori by finding a basis set for the nullspace of $A$. 
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

**Configuration matrix**

**The covariance matrix**

\[(A^T A)\vec{\Gamma} = 0\]

**Existence**: \(\det(A^T A) = 0\)

**Uniqueness**: \(\text{Rank}(A) = N - 1\)
Triangular cell

\[ A = \begin{pmatrix}
A_{231} \left( \frac{1}{l_{21}^2} - \frac{1}{l_{31}^2} \right) & 0 & 0 \\
0 & A_{312} \left( \frac{1}{l_{32}^2} - \frac{1}{l_{12}^2} \right) & 0 \\
0 & 0 & A_{123} \left( \frac{1}{l_{13}^2} - \frac{1}{l_{23}^2} \right)
\end{pmatrix} \]
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Lattices as fixed points
Singular value distribution
Pattern decomposition
Shannon entropy of a lattice

\[ A = \Delta \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix} \]

- \( \Delta \) is the triangle area
- \( a_1 = \left( \frac{1}{l_{21}^2} - \frac{1}{l_{31}^2} \right) \), \( a_2 = \left( \frac{1}{l_{12}^2} - \frac{1}{l_{32}^2} \right) \), \( a_3 = \left( \frac{1}{l_{13}^2} - \frac{1}{l_{23}^2} \right) \).
- \( a_1 \neq a_2 \neq a_3 \): Rank = 3, Nullspace dimension = 0
- Isosceles: Rank = 2, Nullspace dimension = 1
  \[ \vec{\Gamma} = (\Gamma_1, \Gamma_2, \Gamma_3) : \{(1, 0, 0)^T\} \]
- Equilateral: Rank = 0, Nullspace dimension = 3
  \[ \vec{\Gamma} = (\Gamma_1, \Gamma_2, \Gamma_3) : \{(1, 0, 0)^T, (0, 1, 0)^T, (0, 0, 1)^T\} \]
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Triangular cell

- If any of the three are slightly perturbed, or place a fourth point at a randomly chosen position
Triangular cell

- Symmetry is broken and the configuration matrix will generically have full rank hence empty nullspace.

- Although the equilateral triangle is linearly stable, it is not robust.
- Robustness is a property associated with the structure of the configuration matrix.
Singular value decomposition

- The general tool for finding the *optimal* orthogonal basis set for the nullspace of a non-normal ($A^T A \neq A A^T$) matrix is the **Singular Value Decomposition**
- The $N$ singular values, $\sigma^{(i)}$, of the $M$ by $N$ real matrix $A$, are non-negative real numbers that satisfy

$$A \vec{v}^{(i)} = \sigma^{(i)} \vec{u}^{(i)}; \quad A^T \vec{u}^{(i)} = \sigma^{(i)} \vec{v}^{(i)},$$

where $\vec{u}^{(i)} \in \mathbb{R}^M$ and $\vec{v}^{(i)} \in \mathbb{R}^N$. 
Singular value decomposition

- Generalization of the spectral factorization for normal matrices:

\[ A = U\Sigma V^T \]

- \( U \) is an \( M \times M \) orthogonal (i.e. \( U^T U = I \)) matrix whose columns are the vectors \( \vec{u}^{(i)} \)
- \( V \) is an \( N \times N \) orthogonal matrix with columns given by \( \vec{v}^{(i)} \)
Singular value decomposition

- $\Sigma$ is an $M \times N$ matrix with non-negative numbers on the diagonal and zeros off the diagonal

\[ \Sigma = \begin{pmatrix} \sigma^{(1)} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma^{(N)} \end{pmatrix} \]
Singular value decomposition

- The singular values can be ordered so that
  \[ \sigma^{(1)} \equiv \sigma^{(\text{max})} \geq \sigma^{(2)} \geq \ldots \geq \sigma^{(\text{min})} \geq 0 \]
  and one or more may be zero.

- \[
  (A^T A - \sigma^{(i)^2}) \tilde{v}^{(i)} = 0; \quad (A A^T - \sigma^{(i)^2}) \tilde{u}^{(i)} = 0
  \]

- The singular values squared are the eigenvalues of the covariance matrices \( A^T A \) or \( A A^T \) (which have the same eigenvalue structure)
Singular value decomposition

- The left-singular vectors $\tilde{u}^{(i)}$ are the eigenvectors of $AA^T$, and the right-singular vectors $\tilde{v}^{(i)}$ are the eigenvectors of $A^TA$.
- The right singular vectors $\tilde{v}^{(i)}$ corresponding to $\sigma^{(i)} = 0$ form a basis for the nullspace of $A$. 

Lattices as fixed points
Singular value distribution
Pattern decomposition
Shannon entropy of a lattice
Square cell

- Lattices as fixed points
- Singular value distribution
- Pattern decomposition
- Shannon entropy of a lattice
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Lattices as fixed points
Singular value distribution
Pattern decomposition
Shannon entropy of a lattice

$N = 4$: $A$ has banded structure

$$
\begin{pmatrix}
A_{341} & A_{342} & 0 & 0 \\
A_{241} & 0 & A_{243} & 0 \\
A_{231} & 0 & 0 & A_{234} \\
0 & A_{142} & 0 & A_{143} \\
0 & 0 & A_{132} & 0 \\
0 & 0 & 0 & A_{123} \\
0 & 0 & 0 & A_{124}
\end{pmatrix}
$$

P.K. Newton
Vortex lattice theory
Square cell

\[
A = \left( \frac{d^2 - s^2}{2d^2} \right) \Delta \left( \begin{array}{cccc}
1 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 1 \\
0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 \\
\end{array} \right) = \frac{1}{4} \left( \begin{array}{cccc}
1 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 1 \\
0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 \\
\end{array} \right)
\]

where \( \Delta \equiv s^2/2 \) is the area subtended by any three particles and \( d^2 = 2s^2 \).
Square cell

\[ A = U \Sigma V^T \]

\[ \Sigma = \begin{pmatrix} 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0.3536 & 0 & 0 & 0 \\ 0 & 0 & 0.3536 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \]

\[ V = \begin{pmatrix} -0.5 & 0.7071 & 0 & -0.5 \\ 0.5 & 0 & -0.7071 & -0.5 \\ -0.5 & -0.7071 & 0 & -0.5 \\ 0.5 & 0 & 0.7071 & -0.5 \end{pmatrix} \]
Square cell

\[ N = 4: \text{Singular values} \]

\[
(\sigma^{(1)}, \sigma^{(2)}, \sigma^{(3)}, \sigma^{(4)}) = \left( \frac{1}{2}, \frac{1}{2\sqrt{2}}, \frac{1}{2\sqrt{2}}, 0 \right)
\]

- One-dimensional nullspace with basis \((1, 1, 1, 1)\)
- The four vortices must have equal strength
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Lattices as fixed points
Singular value distribution
Pattern decomposition
Shannon entropy of a lattice

\( N = 5 \) (Central vortex)

\[
A = \frac{1}{4}
\begin{pmatrix}
-1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & -1 & 0 \\
1 & -1 & 0 & 0 & 0 \\
1 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 1 & 0 \\
0 & -1 & 0 & 1 & 0 \\
0 & 1 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & 0
\end{pmatrix}
\]
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Lattices as fixed points
Singular value distribution
Pattern decomposition
Shannon entropy of a lattice

\[ V = \begin{pmatrix}
0.7071 & 0 & -0.5 & 0.5 & 0 \\
0 & 0.7071 & 0.5 & 0.5 & 0 \\
-0.7071 & 0 & -0.5 & 0.5 & 0 \\
0 & -0.7071 & 0.5 & 0.5 & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix} \]

\[ \Sigma = \begin{pmatrix}
0.6124 & 0 & 0 & 0 & 0 \\
0 & 0.6124 & 0 & 0 & 0 \\
0 & 0 & 0.5 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix} \]

P.K. Newton
Vortex lattice theory
Square cell

\[ N = 5: \text{Singular values} \]

\[
(\sigma^{(1)}, \sigma^{(2)}, \sigma^{(3)}, \sigma^{(4)}, \sigma^{(5)}) = \left( \frac{\sqrt{3}}{2\sqrt{2}}, \frac{\sqrt{3}}{2\sqrt{2}}, \frac{1}{2}, 0, 0 \right)
\]

- Nullspace is two-dimensional
- Basis set \{\((1, 1, 1, 1, 0)^T, (0, 0, 0, 0, 1)^T\}\) (as indicated by the two rightmost columns of \(V\))
- Any linear combination of a central vortex with equal strength vortices on the four corners will form an equilibrium.
Decomposing the pattern
What do the other singular values tell us?

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

\[
\hat{\lambda}(i) = \frac{\lambda(i)}{\sum_{j=1}^{N} \lambda(j)}
\]

can be interpreted as probabilities $P_i = \hat{\lambda}(i)$

- The set of numbers $P_i (i = 1, \ldots, N)$ can be thought of as a discrete probability distribution that characterizes the lattice
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Lattices as fixed points
Singular value distribution
Pattern decomposition
Shannon entropy of a lattice

Shannon entropy of the lattice

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

Provides a measure of the distribution of the magnitudes across all the states
• If all energy is clustered in one state:

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

Entropy is minimized (extreme clustering in one state)

• e.g.

\[
A = \begin{pmatrix}
1 & 0 & \ldots & 0 & 0 \\
0 & 0 & \ldots & 0 & 0 \\
0 & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & 0 & 0
\end{pmatrix}
\]

\[ A^T A = A \] has rank one and nullspace dimension \( N - 1 \).
• If the probabilities are all equal:

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

\[ H = \ln N \]

Entropy is maximized (no preferred clustering)

• Every orthogonal matrix \((A^T = A^{-1})\) is a maximum entropy matrix since \(A^T A = AA^T = I\), which implies \(\lambda_i = 1\), \(\hat{\lambda}_i = 1/N\), \((i = 1, \ldots, N)\).

\[
A = \begin{pmatrix}
1 & 0 & \ldots & 0 & 0 \\
0 & 1 & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & 0 & 1
\end{pmatrix}
\]
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Lattices as fixed points
Singular value distribution
Pattern decomposition
Shannon entropy of a lattice

maximum entropy distribution
Distributions that drop-off sharply from the maximum are lower entropy configurations than those that are relatively flat around the maximum.
Comparison of square and square with center vortex

- $N = 4$: Entropy = $\frac{3}{2} \ln 2 = 1.0397$
- $N = 5$: Entropy = $\frac{7}{4} \ln 2 - \frac{3}{4} \ln 3 = 0.3890$
- Square without center vortex has higher entropy, i.e. more equal distribution of energy among modes.
Lattice size

- Frobenius norm
  \[ \|A\|_F^2 = (\sigma^{(1)})^2 + (\sigma^{(2)})^2 + \ldots + (\sigma^{(r)})^2 \equiv \text{trace}(A^T A) \]
- 2-norm \( \|A\|_2 = \sigma^{(1)} \)
- Square: \( \|A\|_F = \frac{1}{\sqrt{2}} \); \( \|A\|_2 = \frac{1}{2} \)
- Square with center: \( \|A\|_F = 1; \quad \|A\|_2 = \frac{\sqrt{3}}{2\sqrt{2}} \)
- Lattice spacing:
  \[ \|A_1 - A_2\|_F^2 \]
- Kullback-Leibler divergence:
  \[ D_{KL}(P, Q) = \sum_{i=1}^{N} P_i \ln \frac{P_i}{Q_i} = H(P, Q) - H(P) \]
Brownian ratchet scheme

- Lattice density: standard theorem (Golub & Van Loan) that the set of full rank matrices are dense in $\mathbb{R}^{M \times N}$, while the set of rank-deficient matrices are not.
- Randomly deposit $N$ points in the plane in an unbiased way and compute the $N$ singular values of the configuration matrix $A$.
- These can be ordered and denoted
  \[ \sigma_1 \equiv \sigma_{(\text{max})} \geq \sigma_2 \geq \ldots \geq \sigma_N \equiv \sigma_{(\text{min})} \geq 0. \]
- The minimum singular value, $\sigma_N$, is positive, with probability one;
Brownian ratchet scheme

To home in on an equilibrium:

• Each point executes an unbiased random walk in $\mathbb{R}^2$
• Compute the singular values of $A$ at each step.
• Keep the new arrangement if the minimal singular value decreases from that of the previous step. Otherwise discard the configuration.
• When $\sigma_N^{(n+1)}$ is below a certain pre-determined threshold, the algorithm has converged.
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Brownian ratchet scheme
Brownian ratchet scheme
Brownian ratchet scheme

![Diagram of Brownian ratchet scheme](image-url)
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Brownian ratchet scheme

Convergence properties of the scheme
Brownian ratchet scheme

$N = 6$: Converged state may not be near initial state
Brownian ratchet scheme

$N = 8$: Nearby converged state
Brownian ratchet scheme

\[ N = 10: \text{Two different converged states with same initial configurations} \]
Brownian ratchet scheme

The lattices found this way all seem to be asymmetric - why?

• Maybe there are no ‘paths’ from an asymmetric initial configuration to a symmetric state?
• Maybe there are no ‘paths’ from an asymmetric initial configuration to a symmetric state? — No

P.K. Newton
Vortex lattice theory
Brownian ratchet scheme

Using the ratchet in reverse allows us to find a path from a given state to a specific initial distribution.
Brownian ratchet scheme

Maximum entropy theory:

- Consider the Shannon entropy of the minimum entropy ($H = 0$) and maximum entropy ($H = \log N$) examples discussed earlier.
- Given $N$, imagine all possible arrangements of $N$ balls in $N$ bins, each bin representing one of the singular values and the number of balls in a bin representing its magnitude.
- There are $N$ arrangements of balls that are clustered in one bin (minimum entropy)
- There are $N!$ arrangements of balls that are spread one ball per bin (maximum entropy)
• This means that the maximal entropy state is overwhelmingly more likely to be picked than the minimal entropy state, particularly as N gets large

Conjecture

Asymmetric states have, on average, higher entropy (better distribution of energy among the svd modes) than symmetric ones (clustered distribution)

• Square lattice favored over square with center since it has higher entropy
• We think there is a connection between maximal entropy states and robust states since generic perturbations increase entropy
Brownian ratchet scheme

Ensemble average comparisons

P.K. Newton            Vortex lattice theory
Brownian ratchet scheme

\[ N = 4 : \text{Regular polygon has higher entropy (more robust) and lower energy (if all strengths are equal).} \]
$N = 5$ Regular polygon has higher entropy (more robust) and lower energy (if all strengths are equal).
Singular value distribution not like random matrices

Filled: Distribution of singular values associated with equilibrium configurations \((N = 6)\)

Unfilled: Random Wishart distribution
The spherical shell model

4

P.K. Newton
Vortex lattice theory
Navier-Stokes equations

\[ u_t + u \cdot \nabla u = -\nabla p + \frac{1}{Re} \Delta u; \quad u(x, 0) = u_0 \]

\[ \nabla \cdot u = 0; \quad Re = \frac{U \cdot L}{\nu} \]

\[ \omega = \nabla \times u \]

\[ \omega_t + u \cdot \nabla \omega = \omega \cdot \nabla u + \frac{1}{Re} \Delta \omega \]

- Large scale motion: \( Re \sim \infty \)
- 2D: \( \omega \cdot \nabla u = 0 \)
Euler equations

\[ \frac{D\omega}{Dt} \equiv \omega_t + \mathbf{u} \cdot \nabla \omega = 0; \quad \omega(x, 0) = \omega_0 \]

\[ \nabla \cdot \mathbf{u} = 0; \quad \omega = \nabla \times \mathbf{u} \]

- Biot-Savart law:
  \[ \mathbf{u}(x, t) = \int \int (\nabla \perp G) (x - y)\omega(y, t)dy \]

- \( G \) is the fundamental solution to Laplace's eqn on the sphere:
  \[ \Delta G = \delta - 1 / \text{surface area} \]
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Atmospheric/Geophysical modeling
Optimal mesh generation using particle methods
Virus structure
J.J. Thomson problem and the plum pudding model

\[ G(\theta, \phi; \theta', \phi') = \delta - \frac{1}{4\pi} \ln(1 - \cos \gamma) \]

• Green’s function: \( G(\theta, \phi; \theta', \phi') \)

\[
\left( \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) \right) G = \delta - \frac{1}{4\pi} \]

• Discrete vorticity representation:

\[
\omega(\theta, \phi; t) = \sum_{i=1}^{N} \frac{\Gamma_i}{2\pi} \delta(\theta - \theta_i(t))\delta(\phi - \phi_i(t))
\]

\[
\int_S \omega dA = 0; \quad \sum_{i=1}^{N} \Gamma_i \neq 0
\]

P.K. Newton
Vortex lattice theory
Discrete Biot-Savart law

\[ \dot{x}_\alpha = \sum_{\beta \neq \alpha}^{N} \Gamma_\beta \left( \nabla_\perp G \right) \cdot (x_\alpha - x_\beta) \quad (\alpha = 1, \ldots, N) \]
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Atmospheric/Geophysical modeling
Optimal mesh generation using particle methods
Virus structure
J.J. Thomson problem and the plum pudding model
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
**Overview of related problems**
Summary
References

**Atmospheric/Geophysical modeling**
Optimal mesh generation using particle methods
Virus structure
J.J. Thomson problem and the plum pudding model
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Atmospheric/Geophysical modeling
Optimal mesh generation using particle methods
Virus structure
J.J. Thomson problem and the plum pudding model

\[ J_1 J_2 ! 1 ! 2 \]

P.K. Newton
Vortex lattice theory
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

Atmospheric/Geophysical modeling
Optimal mesh generation using particle methods
Virus structure
J.J. Thomson problem and the plum pudding model

NOAA GOES7
Hurricane Andrew
1992 Aug 25, 1900 UTC

P.K. Newton
Vortex lattice theory
Icosahedral dissection

FIG. 1. Static icosahedral triangulations of the two-sphere.
Generating accurate finite element meshes for the forward model of the human head in EIT

A. Tizzard et al. (2005)

Table 1. Analysis of FE models.

<table>
<thead>
<tr>
<th></th>
<th>Number of</th>
<th>Number of</th>
<th>Number of</th>
<th>Stretch range</th>
<th>Mean</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>nodes</td>
<td>elements</td>
<td>Stretch</td>
<td></td>
<td>SD below 0.1 (%)</td>
</tr>
<tr>
<td>Standard</td>
<td>5</td>
<td>939</td>
<td>31 111</td>
<td>0.03</td>
<td>0.98</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>688</td>
<td>131 672</td>
<td>0.11</td>
<td>0.99</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>169</td>
<td>136 442</td>
<td>0.08</td>
<td>0.99</td>
</tr>
<tr>
<td>Patient 1</td>
<td>6</td>
<td>935</td>
<td>37 062</td>
<td>0.01</td>
<td>0.99</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>025</td>
<td>48 424</td>
<td>0.02</td>
<td>0.97</td>
</tr>
<tr>
<td></td>
<td>27</td>
<td>959</td>
<td>151 797</td>
<td>0.01</td>
<td>0.98</td>
</tr>
<tr>
<td></td>
<td>29</td>
<td>891</td>
<td>162 753</td>
<td>0.02</td>
<td>0.99</td>
</tr>
<tr>
<td>Patient 2</td>
<td>9</td>
<td>062</td>
<td>47 547</td>
<td>0.02</td>
<td>0.98</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>663</td>
<td>51 043</td>
<td>0.05</td>
<td>0.99</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>799</td>
<td>165 344</td>
<td>0.06</td>
<td>0.99</td>
</tr>
<tr>
<td>Neonate</td>
<td>8</td>
<td>703</td>
<td>45 702</td>
<td>0.02</td>
<td>0.98</td>
</tr>
<tr>
<td></td>
<td>26</td>
<td>586</td>
<td>142 654</td>
<td>0.03</td>
<td>0.99</td>
</tr>
<tr>
<td>Tank</td>
<td>4</td>
<td>882</td>
<td>24 722</td>
<td>0.02</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>959</td>
<td>52 327</td>
<td>0.01</td>
<td>0.98</td>
</tr>
</tbody>
</table>

4. Discussion

The qualities of all the meshes shown in table 1 are generally good. Although there are elements in most of them with stretch values below 0.05, the percentage of these is small and...
Chouraqui & Elber (1996)

(a) Uniform sampling; (b) Spring-mass relaxation; (c) Charged particle equilibria.
$N = 72$: Human polyoma virus (icosahedral symmetry)

X-ray diffraction imaging

Klug & Finch (1965)
An open problem\(^1\) in constrained optimization

- Find extremizers for the Riesz-s energy \(E_s\):

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

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

\(^1\)Proofs of global minimum or best packing only for \(N = 2 - 12\) and \(N = 24\)
Group theoretic approach

FIGURES 15 to 32. The Platonic and Archimedean solids.

P.K. Newton
Vortex lattice theory
How to handle dislocations?

![Diagram of dislocations]

$$N = 932$$  
$$N = 972$$
Summary of interesting issues

- Spectral characterization of lattice structure (large $N$)
- Growth/Formation/Assembly
- Stability/Robustness
- Control/Intervention
Summary of interesting issues

- Spectral characterization of lattice structure (large $N$)
- Growth/Formation/Assembly
- Stability/Robustness
- Control/Intervention
Summary of interesting issues

- Spectral characterization of lattice structure (large $N$)
- Growth/Formation/Assembly
- Stability/Robustness
- Control/Intervention
Recent experiments in Bose-Einstein condensates
Interacting particle formulation
The configuration matrix approach
Brownian ratchet schemes
Overview of related problems
Summary
References

References


