Designer Spin Systems via Inverse Statistical Mechanics

Robert A. DiStasio Jr.

Princeton University, Department of Chemistry, Princeton, New Jersey, USA

IPAM Workshop at UCLA February 27, 2015

< 同 > < 三 > < 三 >

THE INVERSE PROBLEM: PRELIMINARIES

What is the *inverse* problem in statistical mechanics?

・ 回 と ・ ヨ と ・ ヨ と

THE INVERSE PROBLEM: PRELIMINARIES

What is the *inverse* problem in statistical mechanics?

• First the *forward* problem: Given a set of interactions, solve for the structure and equilibrium properties of the system.

$$\Phi(\{\mathbf{R}\},\{V\}) = \sum_{ij} V_2(\mathbf{R}_i,\mathbf{R}_j) + \sum_{ijk} V_3(\mathbf{R}_i,\mathbf{R}_j,\mathbf{R}_k) + \dots$$
$$\Phi(\{\mathbf{R}\},\{V\}) \Rightarrow \{\mathbf{R}\}_{eq}$$

・ 回 ト ・ ヨ ト ・ ヨ ト …

THE INVERSE PROBLEM: PRELIMINARIES

What is the *inverse* problem in statistical mechanics?

• First the *forward* problem: Given a set of interactions, solve for the structure and equilibrium properties of the system.

$$\Phi(\{\mathbf{R}\},\{V\}) = \sum_{ij} V_2(\mathbf{R}_i,\mathbf{R}_j) + \sum_{ijk} V_3(\mathbf{R}_i,\mathbf{R}_j,\mathbf{R}_k) + \dots$$
$$\Phi(\{\mathbf{R}\},\{V\}) \Rightarrow \{\mathbf{R}\}_{eq}$$

• Hence the *inverse* problem: Given a **target** configuration of the system, solve for the optimal set of interactions which will spontaneously produce the desired structure.

$$\Phi(\{\mathbf{R}\},\{V\}) \Leftarrow \{\mathbf{R}\}_{eq}$$

回 と く ヨ と く ヨ と

Applications of the Inverse Problem

• The inverse problem is much more general—conversion of "observables" (obtained via measurement) are transformed into physical information that characterizes a system.

回 とう ほううう ほうし

Applications of the Inverse Problem

- The inverse problem is much more general—conversion of "observables" (obtained via measurement) are transformed into physical information that characterizes a system.
- Inverse problems can be found in many different contexts:
 - *Natural Sciences*: medical imaging, systems biology, population genetics, biochemistry, ...
 - *Physical Sciences*: astronomy, geophysics, statistical mechanics, chemistry, engineering, ...
 - Computer Sciences: pattern recognition, computer vision, machine learning, remote sensing, ...
 - Social Sciences: linguistics, human behavior, economics, archaeology, ...

・ロン ・回 と ・ 回 と ・ 回 と

A BRIEF OVERVIEW OF THE ISING MODEL

- Used to describe the fundamental physics underlying the phenomenon of ferromagnetism in materials.
- The simplest form consists of a two-state (up/down) spin system interacting through a nearest-neighbor potential.
- Spins are usually arranged on a lattice—isomorphic to an array of black/white pixels, the lattice gas model, etc.



THE ISING MODEL: APPLICATIONS

- The Ising model has also been used in many applications:
 - Reconstruction of complex (collective) biological networks of neurons, genes, and proteins.
 - Abnormal cell growth dynamics and tumor formation.

Schneidman, Berry, Segevm, Bialek, Nature (2006). Braunstein, Pagnani, Weigt, Zecchina, J. Stat. Mech. (2008). Torquato, Phys. Biol. (2011).

(日) (日) (日) (日) (日)

THE ISING MODEL: APPLICATIONS

- The Ising model has also been used in many applications:
 - Reconstruction of complex (collective) biological networks of neurons, genes, and proteins.
 - Abnormal cell growth dynamics and tumor formation.
- In addition, the inverse approach applied to the Ising model has many promising applications:
 - Design and reverse engineering of materials with desired spin (magnetic) properties.
 - Study of spontaneous pattern formation in nature.
 - Pattern prediction/recognition and image processing.

Schneidman, Berry, Segevm, Bialek, Nature (2006). Braunstein, Pagnani, Weigt, Zecchina, J. Stat. Mech. (2008). Torquato, Phys. Biol. (2011).

(本部) (本語) (本語) (語)

THE STANDARD/SIMPLEST ISING SPIN MODEL

 One of the simplest Ising models is discretized on a periodic 2-D (square → torus) lattice consisting of N spins with spin projection values of σ_i ± 1.

白 と く ヨ と く ヨ と

THE STANDARD/SIMPLEST ISING SPIN MODEL

- One of the simplest Ising models is discretized on a periodic 2-D (square → torus) lattice consisting of N spins with spin projection values of σ_i ± 1.
- The standard Ising Hamiltonian takes on the following form:

$$\mathscr{H}(J) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j,$$

in which $\langle ij \rangle$ restricts the sum to include only unique pairs of nearest neighbor (*NN*) spins and *J* is the coupling constant.

• The ground states of the ferromagnetic (J = +1) and anti-ferromagnetic (J = -1) NN interactions are well-known (all up/down and the checkerboard).

(ロ) (同) (E) (E) (E)

• In this work, we extend the length of interactions beyond *NN*, but still restrict to a radial two-body potential only, *i.e.*,

$$\mathscr{H}(\{J\}) = -\sum_{i < j} J(R_{ij})\sigma_i\sigma_j,$$

▲□ → ▲ □ → ▲ □ → …

• In this work, we extend the length of interactions beyond *NN*, but still restrict to a radial two-body potential only, *i.e.*,

$$\mathscr{H}(\{J\}) = -\sum_{i < j} J(R_{ij})\sigma_i\sigma_j,$$

• Distances (R_{ij}) and associated degeneracies $(g(R_{ij}))$ are given by the theta series corresponding to a square lattice:

$$heta_3^2(\lambda) = 1 + 4\lambda + 4\lambda^2 + 4\lambda^4 + 8\lambda^5 + 4\lambda^8 + 4\lambda^9 + 8\lambda^{10} + \dots$$

・ 「 ト ・ ヨ ト ・ ヨ ト ・

• In this work, we extend the length of interactions beyond *NN*, but still restrict to a radial two-body potential only, *i.e.*,

$$\mathscr{H}(\{J\}) = -\sum_{i < j} J(R_{ij})\sigma_i\sigma_j,$$

• Distances (R_{ij}) and associated degeneracies $(g(R_{ij}))$ are given by the theta series corresponding to a square lattice:

$$heta_3^2(\lambda) = 1 + 4\lambda + 4\lambda^2 + 4\lambda^4 + 8\lambda^5 + 4\lambda^8 + 4\lambda^9 + 8\lambda^{10} + \dots$$

The solution of the inverse spin problem is attained by finding the optimal set of J(R) that yields a **target** spin configuration as a possible unique (non-degenerate) ground state.

・ 同 ト ・ ヨ ト ・ ヨ ト

 It is now convenient to define the S₂ vector, a quantity closely related to the spin-spin correlation function, <σ_iσ_j>, with components given by:

$$S_2(R) \equiv rac{1}{N} \sum_{i < j} \sigma_i \sigma_j \delta_{R,R_{ij}}.$$

・回 ・ ・ ヨ ・ ・ ヨ ・ …

 It is now convenient to define the S₂ vector, a quantity closely related to the spin-spin correlation function, <σ_iσ_j>, with components given by:

$$S_2(R) \equiv rac{1}{N} \sum_{i < j} \sigma_i \sigma_j \delta_{R,R_{ij}}.$$

 This formalism allows for direct computation of the energy per spin, *ϵ*, via the scalar product of S₂ with J,

$$\epsilon \equiv \frac{E}{N} = -\sum_{R} J(R)S_2(R) = -\mathbf{J}\cdot\mathbf{S}_2.$$

▲圖▶ ▲屋▶ ▲屋▶ ---

 It is now convenient to define the S₂ vector, a quantity closely related to the spin-spin correlation function, <σ_iσ_j>, with components given by:

$$S_2(R) \equiv rac{1}{N} \sum_{i < j} \sigma_i \sigma_j \delta_{R,R_{ij}}.$$

 This formalism allows for direct computation of the energy per spin, *ϵ*, via the scalar product of S₂ with J,

$$\epsilon \equiv \frac{E}{N} = -\sum_{R} J(R)S_2(R) = -\mathbf{J}\cdot\mathbf{S}_2.$$

• $|S_2(R)|$ assumes a maximum value when all spins separated by *R* are aligned or anti-aligned, reflecting the coordination at *R*.

・ 同 ト ・ ヨ ト ・ ヨ ト

• We have developed a competitor-based 0 K optimization scheme that combines both *forward* and *inverse* techniques.

Rechtsman, Stillinger, Torquato, Phys. Rev. E (2006). DiStasio, Marcotte, Car, Stillinger, Torquato, Phys. Rev. B (2013).

白 ト イヨト イヨト

- We have developed a competitor-based 0 K optimization scheme that combines both *forward* and *inverse* techniques.
- Given a target spin configuration, \mathscr{T} , the goal is to find the **shortest-range** potential that favors \mathscr{T} by energetically disfavoring *all possible competitors*.



Mona Lisa (RGB→GS→B/W)

Rechtsman, Stillinger, Torquato, Phys. Rev. E (2006). DiStasio, Marcotte, Car, Stillinger, Torquato, Phys. Rev. B (2013).

高 とう モン・ く ヨ と

- We have developed a competitor-based 0 K optimization scheme that combines both *forward* and *inverse* techniques.
- Given a target spin configuration, \mathscr{T} , the goal is to find the **shortest-range** potential that favors \mathscr{T} by energetically disfavoring *all possible competitors*.



Mona Lisa (RGB→GS→B/W)

• This potential maximizes $\Delta \epsilon^k = \epsilon^{C_k} - \epsilon^{\mathscr{T}}$, the difference between the energetically closest competitor, C_k , and \mathscr{T} , over the entire set of available competitors.

Rechtsman, Stillinger, Torquato, Phys. Rev. E (2006). DiStasio, Marcotte, Car, Stillinger, Torquato, Phys. Rev. B (2013).

▲御▶ ★ 国▶ ★ 国▶ 三日

• Obtaining this potential is achieved via global optimization of *z*, the corresponding objective function:

$$z \equiv \max_{\mathbf{J}} \left[\min_{C_k} \left[\Delta \epsilon^k \right] \right] = \max_{\mathbf{J}} \left[\min_{C_k} \left[-\sum_{R} J(R) \left[S_2^{C_k}(R) - S_2^{\mathscr{T}}(R) \right] \right] \right]$$

DiStasio, Marcotte, Car, Stillinger, Torquato, Phys. Rev. B (2013).

個 と く ヨ と く ヨ と …

• Obtaining this potential is achieved via global optimization of *z*, the corresponding objective function:

$$z \equiv \max_{\mathbf{J}} \left[\min_{C_k} \left[\Delta \epsilon^k \right] \right] = \max_{\mathbf{J}} \left[\min_{C_k} \left[-\sum_{R} J(R) \left[S_2^{C_k}(R) - S_2^{\mathscr{T}}(R) \right] \right] \right]$$

- Subject to the constraints that Δε^k ≥ 0 ∀ k and the set of J(R) are bounded within the interval [-1, +1].
- Since the Δε^k is linear in the {J(λ)}, linear programming (LP) is used to efficiently generate the biasing potential exactly (*i.e.*, to machine precision).

DiStasio, Marcotte, Car, Stillinger, Torquato, Phys. Rev. B (2013).

• **STEP 0**: To initiate the procedure, the target structure and a single competitor are required.

DiStasio, Marcotte, Car, Stillinger, Torquato, Phys. Rev. B (2013).

(日) (日) (日)

3

• **STEP 0**: To initiate the procedure, the target structure and a single competitor are required.

In a sequential loop over the allowed distances $R' \leq R_{max}$:

- STEP 1: LP generates a potential with a maximum extent of R' s.t. ε^𝔅 < ε^{C_k} ∀ k, if this potential exists.
- STEP 2: SA-MC employs this potential to find a new competitor C_{k+1} s.t. ε<sup>C_{k+1} ≤ ε^S, if this competitor exists.
 </sup>
- **STEPS 1** and **2** are then iterated until:
 - For a given $\{C_k\}$, LP is unable to generate a potential that favors \mathscr{T} . **GO TO 1**
 - For a given {*J*(*R*)}, SA-MC is unable to locate a competitor that is lower in energy than \mathscr{T} . **EXIT**

DiStasio, Marcotte, Car, Stillinger, Torquato, Phys. Rev. B (2013).

- ◆ □ ▶ ◆ 三 ▶ ◆ □ ● ● ○ ○ ○ ○

ANALYZING THE SOLUTIONS

• **CLASS I:** Solutions in which a potential was found that generates \mathscr{T} as a *unique* (non-degenerate) ground state up to translations, rotations, reflections, and spin inversion operations.

*Uniqueness is defined here to allow for translations, rotations, reflections, and spin inversion of the target structure.

▲圖 ▶ ▲ 臣 ▶ ▲ 臣 ▶ …

ANALYZING THE SOLUTIONS

- **CLASS I:** Solutions in which a potential was found that generates \mathscr{T} as a *unique* (non-degenerate) ground state up to translations, rotations, reflections, and spin inversion operations.
- CLASS II: Solutions in which a potential was found that generates *S* as a *non-unique* ground state, with degenerate spin configurations having the same S₂ as *S* (S₂-type degeneracies). *Remark*: S₂-type degeneracies remain isoenergetic for *any* choice of the spin-spin interaction potential.

*Uniqueness is defined here to allow for translations, rotations, reflections, and spin inversion of the target structure.

ANALYZING THE SOLUTIONS

- **CLASS I:** Solutions in which a potential was found that generates \mathscr{T} as a *unique* (non-degenerate) ground state up to translations, rotations, reflections, and spin inversion operations.
- CLASS II: Solutions in which a potential was found that generates *S* as a *non-unique* ground state, with degenerate spin configurations having the same S₂ as *S* (S₂-type degeneracies). *Remark*: S₂-type degeneracies remain isoenergetic for *any* choice of the spin-spin interaction potential.
- CLASS III: Solutions that are not contained in either Class I or II as defined above.

*Uniqueness is defined here to allow for translations, rotations, reflections, and spin inversion of the target structure.

・ロト ・回ト ・ヨト ・ヨト

MAPPING SPIN CONFIGURATIONAL SPACE ONTO S_2

$$S_2(R) \equiv \frac{1}{N} \sum_{i < j} \sigma_i \sigma_j \delta_{R,R_{ij}}$$



- Nearest-neighbor S_2 values for select spin configurations.
- The gray shading represents the **entire spectrum** of possible spin configurations discretized on a periodic square lattice.

MAPPING SPIN CONFIGURATIONAL SPACE ONTO S₂



イロン イ部ン イヨン イヨン 三日

TARGET STRUCTURES: STRIPED PHASES

Graphical depiction of the SP[m, n] striped phase spin configuration



- Found in a variety of materials, including magnetic films, monolayers, and liquid crystals.
- Tailoring the electronic and magnetic properties of SP materials has many direct technological applications.
- An understanding of the interactions necessary to generate SP would prove invaluable in the design of striped materials.

Systematic study of n = 1, 2, ..., 10 revealed that all SP[n, n] spin configurations are unique ground states (Class I).

Giuliani, Lebowitz, Lieb, Phys. Rev. B (2006), (2007), (2011).

・ 同 ト ・ ヨ ト ・ ヨ ト …

- Systematic study of n = 1, 2, ..., 10 revealed that all SP[n, n] spin configurations are unique ground states (Class I).
- These finite-range potentials (of length *n*) are discrete by construction and have compact support.
- Alternative to the infinite-range interactions known to generate **SP** comprised of short-range ferromagnetic and long-range anti-ferromagnetic (dipolar-like) interactions.

Giuliani, Lebowitz, Lieb, Phys. Rev. B (2006), (2007), (2011).

・ 同 ト ・ ヨ ト ・ ヨ ト …

TARGET STRUCTURES: BLOCK CHECKERBOARDS

Graphical depiction of the CB[m, n] block checkerboard spin configuration



- Generalizations of the classic anti-ferromagnetic Ising spin configuration, *i.e.*, the *simple* checkerboard (**CB**[1,1]).
- The lattice-gas analogs provide model systems to study varying pore sizes (ion channels, transport proteins, cell membranes, metal organic frameworks).

• With the exception of **CB**[1, 1], a systematic study of n = 2, 3, ..., 10 revealed that all **CB**[n, n] spin configurations are *degenerate* ground states (Class II).

米部 シネヨシネヨシ 三日

- With the exception of **CB**[1, 1], a systematic study of n = 2, 3, ..., 10 revealed that all **CB**[n, n] spin configurations are *degenerate* ground states (Class II).
- Like the SP[n,n] cases, the *shortest* radial interaction potentials are of length *n*.
- As Class II solutions, the **CB**[*n*, *n*] spin configurations have a finite set of *S*₂-degeneracies.

・回 ・ ・ ヨ ・ ・ ヨ ・

 S_2 -type degeneracies for the CB[2, 2] spin configuration.



イロト イヨト イヨト イヨト

æ

 S_2 -type degeneracies for the CB[4, 4] spin configuration. The number of microstates (*clockwise from upper left-hand corner*) is 32, 128, 128, 32.



Robert A. DiStasio Jr.

Designer Spin Systems via Inverse Statistical Mechanics

2

The CB[N,N] Spin Configurations

The number of S_2 -type degeneracies for the **CB**[n, n] spin configurations g(n) was found as:

$$g(n) = 1 + \frac{\lfloor \frac{n}{2} \rfloor \left(\lfloor \frac{n}{2} \rfloor + 1 \right)}{2}$$

from which it is clear that g(n) increases quadratically with n.



Robert A. DiStasio Jr. Designer Spin Systems via Inverse Statistical Mechanics

THE SP[M,N] AND CB[M,N] SPIN CONFIGURATIONS

Solution classes for the SP[m, n] and CB[m, n] spin configurations.

						-	-	-	-	-	-	-	-	-	-			-	_	_	_	_	-	-	-	-	-	-	-	-	
	0	\overline{CI}	255	T	Γ'	1		1			1	1	1	1			0	\overline{CI}	255	I	Γ'			1	1	1					· 1
- 5	Η 🖌	či	200	îп	0	0	0	0	0	0	0	0		0	×	5	H o	či	200	ÎΤ	•	۰	۰	۰	۰	۰	۰		۰	۰	-
	Ľ	CI	a55	m													II		ass	111											
																	L ^	U	ass	ш											
- 1	F			0	0	0	0	0	0	0	0	×		0	_	1	F			0	0	0	0	0	0	0		×	0		_
-				Ť	Ĩ		Ĩ		×.	×.						-					÷.	÷.	÷.	÷.	÷.	÷.			÷.,		
					-									_																	
= 3			0	0	0	0	0	0	×	0	0	×	0	0	×-	≍3	-		•	•	•	•	•	•	×			×			-
2	E -	0	0	0	0	×	0	×		×	0	×	0	×	-	2	F	٥	۵	٥	٥	×	٥	×		×					-
_																-															
1		0													~	1	L	~													
1	·۲	0	<u>^</u>	<u>^</u>	<u></u>	<u> </u>	1	F۲	~	<u>^</u>	<u></u>	<u> </u>																			
		_			1		1		1	1	1	1	1	1	1			1	1		1	1	1				1	1	1	1	1
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
	•	_	-		-	~		ň		- 0							-	_	2	•	-	2	÷	ň		- 0					

- For the $n \neq m$ case, the situation is a bit more complicated...
- Both SP[m, n] and CB[m, n] admit Class III solutions if and only if n/m ∈ Z ≥ 3.
- Indicative of the limitations of a radial pairwise interactions in stabilizing configurations with two distinct length scales.

(4月) (1日) (日) 日

• What types of **target** spin configurations can be generated as unique ground states using radial pairwise interactions?

・ 回 と ・ ヨ と ・ モ と …

- What types of **target** spin configurations can be generated as unique ground states using radial pairwise interactions?
- Are there any "rules of thumb" regarding the solution class corresponding to a given spin configuration?
 - Type and extent of symmetries (order) exhibited by a given spin configuration do not seem to correlate with solution class.

・ 同 ト ・ ヨ ト ・ ヨ ト …

- What types of **target** spin configurations can be generated as unique ground states using radial pairwise interactions?
- Are there any "rules of thumb" regarding the solution class corresponding to a given spin configuration?
 - Type and extent of symmetries (order) exhibited by a given spin configuration do not seem to correlate with solution class.
- Is it safe to assume that the number of Class I solutions will asymptotically tend to zero in the large system limit? What about Class II solutions?

・ 回 と ・ ヨ と ・ ヨ と

Number of spin configurations in each solution class existing on the $n \times n$ square lattice from an exhaustive enumeration of all $2^{n \times n}$ possibilities.

Size	N _I	$N_{\rm II}$	N _{III}	N _{conf}
1×1	1	0	0	2
2×2	3	0	1	16
3×3	3	2	6	512
4×4	5	1	266	65,536
5×5	74	29	8209	33,554,432

• While the number of Class I and II solutions increases with system size, their relative population tends to zero in the same limit.

< 回 > < 注 > < 注 > … 注

NI	N _{II}	N _{III}
28	25	1737
16	4	1690
17	0	1415
4	0	1226
4	0	903
4	0	623
0	0	357
0	0	169
0	0	64
0	0	19
0	0	5
0	0	1
1	0	0
	NI 28 16 17 4 4 0 0 0 0 0 0 10 11	$\begin{array}{c ccc} N_{\rm I} & N_{\rm II} \\ 28 & 25 \\ 16 & 4 \\ 17 & 0 \\ 4 & 0 \\ 4 & 0 \\ 4 & 0 \\ 4 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \end{array}$

• The number of Class I and II solutions also decreases with an increase in the absolute magnetization.

(本部)) (本語)) (本語)) (語)

Is there a correlation between symmetry, complexity, or order and solution class determination?



All 5 × 5 Class I spin configurations (N = 20) that are **not** left invariant under any combination of symmetry operations, displayed left-to-right, top-to-bottom, in order of decreasing absolute magnetization $|\langle \sigma \rangle|$.

イロト イポト イヨト イヨト



All 5 × 5 Class I spin configurations (N = 54) that are left invariant under some combination of symmetry operations, displayed left-to-right, top-to-bottom, in order of decreasing absolute magnetization $|\langle \sigma \rangle|$.

ロ と く 聞 と く き と く き と …

2



All 5 × 5 Class I spin configurations (N = 54) that are left invariant under some combination of symmetry operations, displayed left-to-right, top-to-bottom, in order of decreasing absolute magnetization $|\langle \sigma \rangle|$.

· < @ > < 문 > < 문 > · · 문

PHASES (STATES) OF MATTER



Traditional Criteria

- Homogeneous phase in thermodynamic equilibrium
- Interacting entities are microscopic objects, *e.g.*, atoms, molecules or spins
- Are often distinguished by symmetry-breaking and/or some qualitative change in a bulk property

PHASES (STATES) OF MATTER



Non-Traditional/Broader Criteria

- Reproducible long-lived metastable or non-equilibrium phases, *e.g.*, spin and structural glasses
- Interacting entities need not be microscopic, can include larger building blocks, *e.g.*, colloids and metamaterials
- Endowed with unique properties

イロト イポト イヨト イヨト

NEW PHASES (STATES) OF MATTER



- Let Ω be a spherical window of radius R in \mathbb{R}^d and $\sigma^2 \equiv \langle N^2(R) \rangle \langle N(R) \rangle^2$ be the **number variance**.
- For Poisson and many disordered point patterns: $\sigma^2 \sim R^d$.

NEW PHASES (STATES) OF MATTER



- Let Ω be a spherical window of radius R in \mathbb{R}^d and $\sigma^2 \equiv \langle N^2(R) \rangle \langle N(R) \rangle^2$ be the **number variance**.
- For Poisson and many disordered point patterns: $\sigma^2 \sim R^d$.
- Hyperuniform point patterns: σ^2 grows slower than R^d .
 - Infinite-wavelength density fluctuation vanish.
 - Implies that $S(\mathbf{k}) = \frac{1}{N} \left| \sum_{j=1}^{N} \exp[i\mathbf{k} \cdot \mathbf{r}_j] \right|^2 \to 0$ as $\mathbf{k} \to 0$.

イロト イポト イヨト イヨト

ALL CRYSTALS ARE TRIVIALLY HYPERUNIFORM



- All perfect crystals are hyperuniform in that $\sigma^2 \sim R^{d-1}$.
- The degree to which they suppress large-scale density fluctuations varies.

WHICH POINT PATTERN IS HYPERUNIFORM?





- 4 回 2 - 4 □ 2 - 4 □

WHICH POINT PATTERN IS HYPERUNIFORM?



- Characterized by "hidden order" on long/large length scales.
- Examples of hyperuniform systems in nature: ultracold gases of atoms, avian cone photoreceptors.

Hyperuniform Avian Cone Receptors



- Not located on the "ideal" triangular lattice as found in insects and some fish.
- Each of the 5 cones form disordered/irregular patterns that are hyperuniform (*i.e.*, forming a multi-hyperuniform system).

Jiao, Corbo, Torquato, Phys. Rev. E (2014).

Hyperuniform Avian Cone Receptors



- Not located on the "ideal" triangular lattice as found in insects and some fish.
- Each of the 5 cones form disordered/irregular patterns that are hyperuniform (*i.e.*, forming a multi-hyperuniform system).

ALL STEALTHY PATTERNS ARE HYPERUNIFORM



- "Stealthy" point patterns take hyperuniformity one step further and are characterized by S(k) = 0 for 0 < k ≤ K.
- Applications include the design of photonic devices with large complete band gaps and color sensors.
- Concept can also be extended to S(k) = 0 for K₁ < k ≤ K₂ for selective suppression of radiation absorption.

DO DISCRETE DISORDERED STEALTHY PATTERNS EXIST?

To answer this question, we first turned to exhaustive enumeration of the point patterns discretized on the periodic 2-D lattice...



- Limited to small system sizes (6 \times 6 \Rightarrow 2^{36} configurations).
- Order/Disorder metric based on signature of disordered continuous systems (*e.g.*, ideal gas)...

DO DISCRETE DISORDERED STEALTHY PATTERNS EXIST?

Can we efficiently generate larger disordered stealthy patterns?



• Simulated Annealing (MC) with the following fictitious energy:

$$\theta = \sum_{\mathbf{k} \leq \mathcal{K}} \left[S(\mathbf{k}) - S^{\mathscr{T}}(\mathbf{k}) \right]^2 = \sum_{\mathbf{k} \leq \mathcal{K}} \left[S(\mathbf{k}) - 0 \right]^2 = \sum_{\mathbf{k} \leq \mathcal{K}} \left[S(\mathbf{k}) \right]^2$$

• Efficient and works best for small K and low concentrations.

CONCLUSIONS AND FUTURE WORK

- In this work, we developed a competitor-based 0 K optimization scheme which provides a general framework in which one can attack the inverse problem.
- This algorithm was systematically applied in the study of several fundamental spin patterns (**SP** and **CB**) as well as in a general enumeration study on the 2D square lattice.
- Also presented were some preliminary results proving computational evidence of the existence of discrete and disordered stealthy/hyperuniform patterns.
- It would be interesting to utilize these approaches in the design of novel materials with desired properties.

(日本) (日本) (日本)

Acknowledgments



Frank Stillinger



Salvatore Torquato







Roberto Car

Étienne Marcotte

Ge Zhang

Robert A. DiStasio Jr. Designer Spin Systems via Inverse Statistical Mechanics

POSTDOC OPPORTUNITIES AT CORNELL UNIVERSITY



Several positions are available for talented and highly motivated postdoctoral researchers in my research group in the Department of Chemistry and Chemical Biology at Cornell University. Contact me at distasio@cornell.edu for more details.

イロト イヨト イヨト イヨト